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Review and future research directions

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Review

Water quality modeling in sewer networks: Review and future research directions

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ABSTRACT

Urban sewer networks (SNs) are increasingly facing water quality issues as a result of many challenges, such as population growth, urbanization and climate change. A promising way to addressing these issues is by developing and using water quality models. Many of these models have been developed in recent years to facilitate the management of SNs. Given the proliferation of different water quality models and the promise they have shown, it is timely to assess the state-of-the-art in this field, to identify potential challenges and suggest future research directions. In this review, model types, modeled quality parameters, modeling purpose, data availability, type of case studies and model performance evaluation are critically analyzed and discussed based on a review of 110 papers published between 2010 and 2019. The review identified that applications of empirical and kinetic models dominate those of data-driven models for addressing water quality issues. The majority of models are developed for prediction and process understanding using experimental or field sampled data. While many models have been applied to real problems, the corresponding prediction accuracies are overall moderate or, in some cases, low, especially when dealing with larger SNs. The review also identified the most common issues associated with water quality modeling of SNs and based on these proposed several future research directions. These include the identification of appropriate data resolutions for the development of different SN models, the need and opportunity to develop hybrid SN models and the improvement of SN model transferability.

1. Introduction

Sewer networks (SNs), or wastewater networks, are considered to be one of the most important urban infrastructure systems, as they play a vital role in ensuring public health and safety, protecting the urban water environment, preventing the spread of waterborne diseases, and reducing the risk of urban floods (Vollertsen et al., 2011; Barone et al., 2019; Pikaar et al., 2014). SNs are typically composed of pipes, manholes, pumping stations, overflow structures and other hydraulic facilities that are normally buried underground (Joseph-Duran et al., 2014) and represent significant infrastructure investments. For example, the value of sewer pipes is estimated to be up to $1 trillion USD in the USA (Pikaar et al., 2014) and $35 billion USD in Australia (Jiang et al., 2016).

Historically, SNs have been designed to collect wastewater and

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stormwater, transporting them to wastewater treatment plants (WWTPs) for processing or disposal (Martin and Vanrolleghem 2014; Haghighi and Bakhshipour 2015). Such SNs are generally referred to as combined sewer systems (CSSs), as they transport a combination of wastewater and stormwater (Hager and Gisonni 2005). However, many cities have separated or are separating CSSs into independent storm drainage systems (storm sewers or infiltrations facilities) and foul sewer systems (Thorndahl et al., 2015, Mahaut and Andrieu, 2018), where the former are used to convey urban runoff solely to surface waters (e.g., rivers) and the latter are used to deliver sewerage that is collected from houses and commercial buildings before being conveyed to treatment facilities. This separation can be beneficial to urban water environments as it can avoid combined sewer overflows (CSO, Joseph-Duran et al., 2015; Mollerup et al., 2015). However, illicit connections between storm drainage and sewer systems are often observed in many cities with separate systems, causing storm water to be polluted with sewage or foul sewers to be hydraulically overloaded due to infiltration and inflow (I/I) (Panasiuk et al., 2016).

1.1. Drivers of change

Over the past few decades, sewer networks (SNs) have been subject to significant changes due to a number of drivers, including, for example, population growth, climate change, system changes, variation of pollutant discharge patterns, human activities, as well as the emergence of new technology and changing regulations, as shown in Fig. 1. More specifically, population growth and climate change can substantially increase the amount of wastewater to be delivered (Egger and Maurer 2015; Sweetapple et al., 2018). Resulting system changes are often represented by the expanded spatial scales of SNs, increased complexity in their topology structures and system ageing (Rokstad and Ugarelli 2015; Huang et al., 2018). The nature of the wastewater to be treated is also changing, with increases in wastewater concentrations due to water conservation (Bailey et al., 2020), separation at source and other related measures (discharge pattern variations, Lyu et al., 2016). The amount and type of harmful pollutants that cannot be easily removed at WWTPs is also likely to increase as the number of new substances keeps growing. These include, for example, medicine discharges used by an aging population, widely used personal care products, and heavy metals released from industrial activities (Marleni et al., 2012). In addition, regulations about the quality of the water that can be discharged into the environment are becoming more stringent in many countries, such as China (Zhang et al., 2015).

The abovementioned drivers pose significant challenges/difficulties to the effective management and operation of SNs. These challenges can be divided into two main categories, involving those related to system hydraulic capacity, such as pipe and pump sizing (Steele et al., 2016; Tian et al., 2018), and those related to water quality, such as illegal discharges, corrosion, illicit connections, hazard gas production and leaks (Banik et al., 2017; Grengg et al., 2018; Guerineau et al., 2014; Mannina et al., 2018). The focus of this review paper is on the latter challenge-that is, water quality issues in urban SNs. It is also noted that the SNs in this review can be foul sewers, combined sewer systems, gravity sewers, as well as pressurized transport mains, as long as models have been developed to simulate the water quality parameters in these systems.

1.2. Water quality issues

Due to the SN changes as a result of the drivers discussed in Section 1.1, a number of water quality issues occur frequently in many SNs, as illustrated conceptually by a physical system in Fig. 1. As shown, illicit discharges from local businesses can significantly affect water quality in SNs and consequently induce contamination of the receiving water body (McCall et al., 2016). This is because such discharges often contain toxic substances (e.g., heavy metals) that are commonly beyond the processing capacity of downstream WWTPs (Banik et al., 2017; Irvine et al., 2011). Another water quality issue within SNs is deposits, e.g., sediments, or fat, oil and grease-FOG (Roushangar and Ghasempour 2017; Song et al., 2018; Yousefelahiyeh et al., 2017). These can induce various water quality issues as a result of their direct impacts on flow capacities, such as manhole overflows (Hager and Gisonni 2005).

Gas emissions (including greenhouse and poisonous gases) resulting from biochemical reactions in sewer pipes (Auguet et al., 2016) are another typical problem associated with SNs, leading to odour issues. These hazardous gases not only affect the air quality of surrounding areas, but can also dissolve in the wastewater and hence can threaten the safety of sewer systems, e.g., via pipe erosion or explosion (Grengg et al., 2018). As shown in Fig. 1, leaks from sewer pipes are also frequently reported in many studies, which can be due to pipe failures, inadequate sealing or illicit connections (Beheshti and Saegrov 2018). These leaks can result in exfiltration of wastewater when the groundwater tables are below sewer invert level (Du et al., 2013), and can also induce infiltration of groundwater if the groundwater tables are high (Divers et al., 2013). These exfiltration or infiltration issues can significantly affect surrounding environments (Lee et al., 2015) or influence the operation

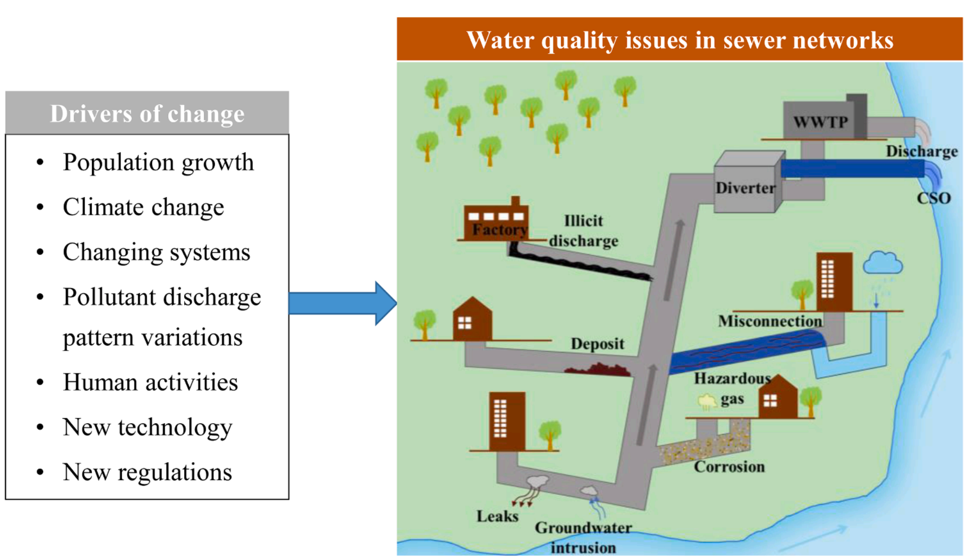

Fig. 1. Schematic illustration of the motivation for this review.

of WWTPs (Ganora et al., 2017; Karpf and Krebs 2013). Another potential problem is the illicit connection between sewer and stormwater pipes for separated SNs (foul sewers). Such issues are reported frequently in many developing countries, such as China (Montserrat et al., 2015; Xu et al., 2016). A recent survey reports that the COD concentrations of the inflows of 70% of WWTPs in China are less than 300 mg/L due to unexpected infiltration and inflows (Xu et al., 2016), highlighting the widespread nature of this issue.

1.3. Importance of water quality modeling in SNs

To address the issues highlighted in Fig. 1, significant research efforts have been devoted to understanding the underlying mechanisms and processes that cause these issues, such as the underlying reaction processes of gas emissions (Liu et al., 2015a). The majority of these studies are based on laboratory experiments or real system samples taken at specific locations (Xu et al., 2016). While these studies have made significant contributions to enable an improved understanding of biochemical processes, they are insufficient to allow for the effective management and operation of entire SNs. This is mainly because the majority of SNs are distributed over a large spatial area with pipes buried underground and hence it is difficult, if not impossible, to collect data or undertake experiments for all locations of these systems to comprehensively understand the changes in various water quality parameters.

A promising way of addressing this issue is via water quality models. Such models provide, at least theoretically and indicatively, insights into potential issues over the full spatial extent of SNs, as well as how these might change in response to the drivers of change discussed in Section 1.1, conditioned on the improved understanding of the underlying reaction processes of the water quality parameters that can be achieved from limited experiments. This provides an opportunity to develop effective and efficient system management and operational strategies for SNs (Gao et al., 2018), as well as the development of plans for the future. The demand for water quality modeling has increased in recent years, as real-time system management and operation are becoming more important in the domain of SNs (Kiilerich et al., 2018). This is partly driven by rapid developments in sensor and information technologies (Zheng et al., 2018), which can assist with real-time data acquisition, transmission, and storage, all of which can be used to calibrate and validate existing water quality models, as well as to develop new models.

1.4. Motivation for this review

As stated above, a number of water quality issues exist within SNs (Section 1.2) as a result of the drivers of change shown in Fig. 1. Attempts have been made to address these issues with the aid of water quality models due to their significant potential for addressing some of these problems, as mentioned in Section 1.3. This is supported by the fact that a broad range of water quality parameters has been modeled using different techniques over the past 10 years (between 2010 and 2019). However, to the best of our knowledge, there is a lack of a critical and comprehensive review to provide knowledge on the current status of modeling across different water quality parameters and the issues associated with current modeling practice, to provide the articulation of the most fruitful directions to enable this field of research to progress as effectively as possible. While a number of previous reviews are available (e.g., Eijo-Rio et al., 2015, Liu et al., 2015b, Shammay et al., 2016, Talaiekhozani et al., 2016, Carrera et al., 2016, Jiang et al., 2017), they have mainly focused on specific water quality parameters, especially on the transmission processes and control methods of water quality parameters, rather than the development of water quality modeling techniques (the focus of the present review). Consequently, this review provides new knowledge into the potential challenges/issues associated with existing water quality modelling of SNs, and provides guidance on the future development of water quality modeling techniques.

In summary, the overall objective of this paper is to review the progress of developing and using models for various SN quality parameters, rather than a particular model type or a specific water quality type. In addition, the common issues and future directions associated with various water quality models are identified. The specific objectives of this review (See Fig. 1) include providing: (i) a comprehensive summary of the current status of water quality modeling for SNs, where water quality parameters, model purpose, data availability, model applications (case studies) and model performance evaluation associated with different model types are analyzed critically, (ii) a detailed discussion on potential challenges/issues associated with models applied to water quality parameters within SNs; and (iii) horizon scanning outcomes and identification of future research needs and directions in relation to water quality modeling in SNs.

The remainder of this paper is structured as follows. Section 2 articulates the review methodology adopted in this study. Section 3 provides a detailed and critical review of current water quality models, and Section 4 presents a comprehensive analysis of the challenges/issues associated with existing water quality modelling methods. Finally, future directions in this research are discussed in Section 5.

2. Review methodology

In this review, we have identified 110 publications published over the past 10 years (2010–2019), which are associated with water quality models applied to the domain of sewer networks (SNs). It is expected that such a review time period is sufficient to represent the overall state-of-the-art progress of water quality modeling in SNs. These papers are identified using the following steps. Firstly, “sewer systems”, “sewer networks”, “sewer pipes”, “foul sewers”, “wastewater networks” and “drainage systems” are used as keywords to search for papers in the Web of Science database (Thomson Reuters, 2016). Secondly, a review of the abstracts of these papers is conducted to identify the papers that are relevant to water quality modeling, identifying 97 papers to be included in this review. Finally, the authors used the above keywords to search across a number of influential wastewater-related journals and conference proceedings (e.g., International Conference on Urban Drainage Modeling), including Water Research, Water Resources Research, Journal of Hydrology, Environmental Modeling and Software, Journal of Water Resources Planning and Management, Hydrology and Earth System Sciences and Water Science and Technology, leading to the inclusion of an additional 13 papers. Consequently, a total of 110 publications are identified for review.

It is noted that it is difficult, if not impossible, to ensure all the published papers between 2010 and 2019 regarding SN water quality modelling have been included in this review. This may have a certain impact on the observations regarding some particular model properties (e.g., the model purposes in Section 3.3). However, it is believed that the main progress, as well as the main characteristics of the SN water quality models, can be identified based on the selected 110 papers.

3. Current status of water quality modeling in SNs

Fig. 2 provides a conceptual representation of the factors considered in our critical review of the status of water quality modeling within SNs. These factors are selected for review as they represent the main steps involved in model development and application. As shown in this figure, a model type (Section 3.1) needs to be selected for a particular problem when developing models for particular water quality parameters (Section 3.2). This is followed by the analysis of model purpose (e.g., prediction, process understanding and control, Section 3.3) and the availability of the data (Section 3.4) that are used for model development, such as data collection frequency (e.g., continuous or grab sample) and data type (e.g., real or experimentally generated). Finally, the properties of the case studies (e.g., laboratory based or real system,

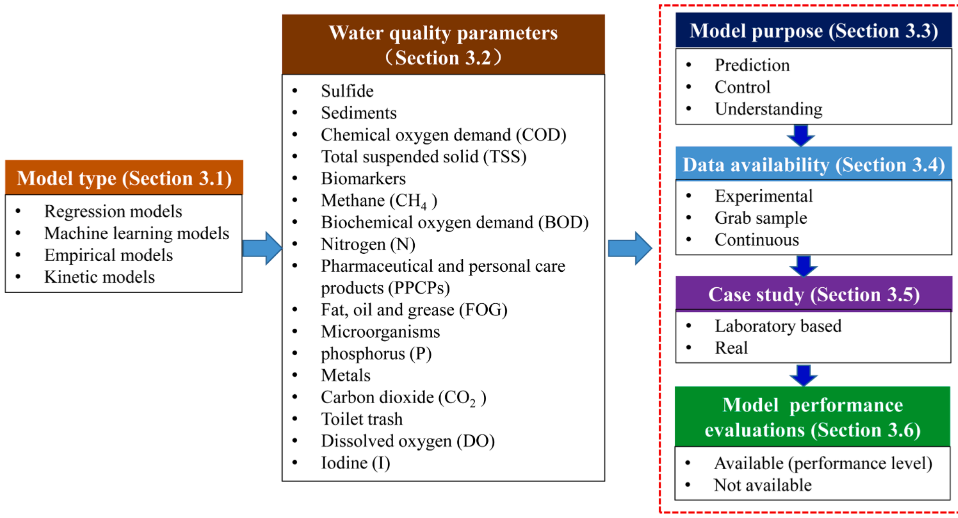

Fig. 2. Conceptual representation of the factors considered in the critical review.

Section 3.5) to which the models have been applied and the resultant model performance (Section 3.6) are reviewed. It is noted that model performance evaluation is not conducted for individual papers, but focuses on the trends emerging across the papers considered.

3.1. Modeling approaches used

Based on a detailed review, four different model types have been identified based on their structure properties, which are regression models, machine learning models, empirical models and kinetic models. It should be noted that, while several classifications are possible, the models of the reviewed papers have been grouped into four different types whereas these models represent a spectrum of model types on a continuum (Mount et al., 2016; Langeveld et al., 2017; Brepols et al., 2019). More specifically, both regression and machine learning models are data-driven model types, but they are based on different model structures and philosophies. Regression models, as a simple type of data-driven models with pre-specified model structures, have been often used to describe the relationships between water quality parameters within SNs and other system properties (e.g., diameters and flow velocity, Shepherd et al., 2010; Safari and Mehr 2018). In addition to regression, machine learning models with unknown model structures ('black box') have also been proposed to analyze the behaviour of water quality parameters within SNs in recent years (Najafzadeh et al., 2017). A few stochastic approaches (Coutu et al., 2016; Roni et al., 2019) developed in the reviewed papers use either regression or unspecified model structures. Therefore, in this study the approaches associated with regression structures are assigned to the regression model type, and approaches with unspecified model structures are assigned to machine learning model type.

In parallel to the development of data-driven models, empirical and kinetic models have also been used for sewer water quality modeling, benefitting from their capacity for representing the transformation processes involving water quality parameters in SNs explicitly (Morales et al., 2016; Li et al., 2018). In empirical models, the water quality parameters are described as a function of a set of environmental parameters, with model structures (which are usually significantly more complex than regression models) as well as parameters often determined by comprehensive experiments (Langeveld et al., 2013; Chaosakul et al., 2014; Matias et al., 2018). In kinetic models, the temporal or spatial changes in water quality parameters are expressed mathematically as a function of their concentrations and a set of decay coefficients (Rudelle et al., 2013; Sun et al., 2018; Zan et al., 2019).

Fig. 3 shows the relative prevalence of the four model types that have been used in the selected papers. As shown in this figure, the use of empirical models (52%) dominates over the use of the other three model types, and the kinetic models (27%) are significantly more frequently used compared to the regression (11%) and machine learning (10%) models. This can be mainly attributed to the following facts: (i) both empirical and kinetic models typically possess greater model transparency and generalization ability than regression and machine learning models, as they are developed (at last partly) according to the physics and chemistry of the analyzed water quality phenomenon based on data from laboratory conditions or field monitoring (Li et al., 2019), thereby facilitating their wide applications in engineering practice; (ii) empirical models often consider the impacts of environmental factors within their model structures explicitly, and hence they can be relatively more easily generalized for various practical applications under different environmental conditions compared to kinetic models that involve environmental influences implicitly; (iii) regression and machine learning models often require a large amount of data for model development, but intensive water quality measurements in SNs are typically difficult and expensive (Zheng et al., 2018).

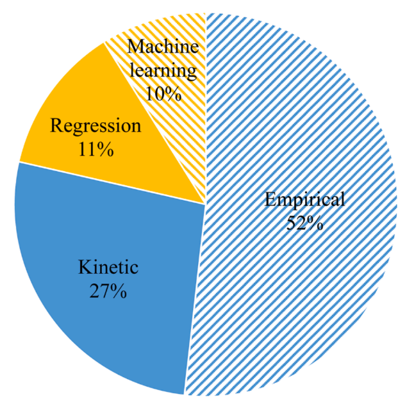

Fig. 3. Relative prevalence of the four model types that have been used in the reviewed papers.

An important feature of these empirical and kinetic models is that they typically combine water quality and hydraulic models, where the latter are used to provide hydraulic variables to enable the simulations of the former (Matos et al., 2019). The reason for this is that the mixing process (involving both advection and dispersion) as well as sedimentation and resuspension (i.e. the transport of different substances by water flow) tend to dominate the water quality processes in SNs.

3.2. Water quality parameters modeled

Fig. 4 shows the number of papers that have modeled different water quality parameters. This figure indicates that sulfide has been the most frequently modeled parameter (in 27 of the 110 papers considered), followed by sediments (25 papers), COD (14 papers) and total suspended solids (TSS) (14 papers). This can be partly explained by the fact that these water quality parameters are closely related to common or important issues within SNs, such as material degradation or odour issues (e.g., H_2S, Carrera et al., 2017), deposit problems (sediments, Montes et al., 2019, 2020) and illicit discharges or inflows (high CODs and TSSs, Xu et al., 2016). Attempts have also been made to model the behaviours of the biomarkers, methane (CH_4), BOD, nitrogen (N), PPCPs, and FOG, as they are typical parameters that characterize overall wastewater quality in sewer pipes (e.g., *N* and *P*, Marleni et al., 2015b). Models have also been developed for microorganisms, phosphorus (P), metals, CO_2, domestic gross solids (DGSs), dissolved oxygen (DO) and Iodine (I), as shown in Fig. 4, but with relatively fewer applications compared to the other quality parameters mentioned above.

The distribution of the four typical modeling approaches used (Fig. 3) across the different water quality parameters modeled is also shown in Fig. 4. As can be seen, empirical or kinetic models have been exclusively used for a range of different water quality parameters, which are the biomarkers, BOD, *N, P*, metals, domestic gross solids (DGSs), dissolved oxygen (DO) and Iodine (I). This can be attributed to the fact that data collection for these complex water quality parameters can be very difficult and hence empirical or kinetic models are preferred, as they require a relatively smaller amount of data for model development. As shown in Fig. 4, regression or machine learning models have been used for the modeling of sulfide, sediments, COD, TSS, CH_4, PPCPs, FOG and microorganisms. Interestingly, CO_2 is the only water quality parameter that has not been modeled using an empirical or kinetic approach, with only regression models being used. Another interesting observation from Fig. 4 is that ANN models have only been frequently developed for sediments (Ebtehaj and Bonakdari, 2014b, 2016). This could be because the development of ANNs typically requires a larger number of data observations, which are generally more available for sediments compared to many other water quality parameters, such as biomarkers, metals and COD (Zan et al., 2019; Kim et al., 2019).

Table 1 provides details of the modeling approaches used for each water quality parameter, including the processes, inputs and outputs considered for each of the models. For example, as shown in this table, when considering sulfide as the quality parameter, two main processes have been modeled. These are the production of sulfide within the SNs under different environmental conditions or impacted by different covariates (e.g., temperature, chemical dosage, Jiang et al. 2010, Alani et al. 2014) and the mass transfer (e.g., H_2S) between the wastewater in SNs and the air under various air velocities (Matias et al., 2018; Teuber et al., 2019). For the regression models of sulfides, the covariates (i.e., inputs) can vary ranging from sewer structure and seasons to wastewater characteristics and chemical dosages, and the model outputs can be H_2S emission hotspots (Zuo et al., 2019) or sulfide concentrations (Jiang et al., 2011). Similar observations can be made for the ANN models applied to sediments, with covariates including pipe sizes, slopes, sediment sizes, sediment concentrations and deposit thickness, and outputs including blockage locations, Froude number or critical flow velocity (Safari and Mehr, 2018; Safari, 2019). It is anticipated that the comprehensive details given in Table 1 can provide significant knowledge regarding the similarities and differences of the modeling processes, model inputs, and model outputs of each model type applied to water quality parameters, which is a useful contribution to the literature.

3.3. Purposes of models

The purposes for which the models were developed are summarized in Fig. 5, where the ratio of different modeling purposes relative to the total number of reviewed papers is presented. As can be seen, models have been developed for three purposes, including prediction, understanding and control. Prediction is a typical aim of many water quality models, where the future behaviours of the quality parameters (e.g., concentrations) are predicted based on the known status of the covariates, as well as the revealed relationship between the covariates and the quality parameters (e.g., regression) being considered (Chaosakul et al., 2014; Campisano et al., 2019). Understanding is often attained by using a process-driven modeling approach, as this enables the underlying temporal and spatial dynamics/evolutions of the water quality parameters within SNs to be determined as a function of varying external conditions (Sharma et al., 2014; Li et al., 2018). Control can be defined as the interventions adopted to influence the behaviour of water quality parameters, mainly through manipulating the factors that can affect their reaction processes (Morales et al., 2016; Guo et al., 2019). It should be noted that within the system controlling processes, the prediction of the status is often required for some specific control strategies, such as predictive control and feedforward control (Langeveld et al., 2013; Liu et al., 2016a). This implies that the prediction and control purposes can be inherently integrated to enable the practical application for some cases. In this study, such an integrated modeling approach is considered

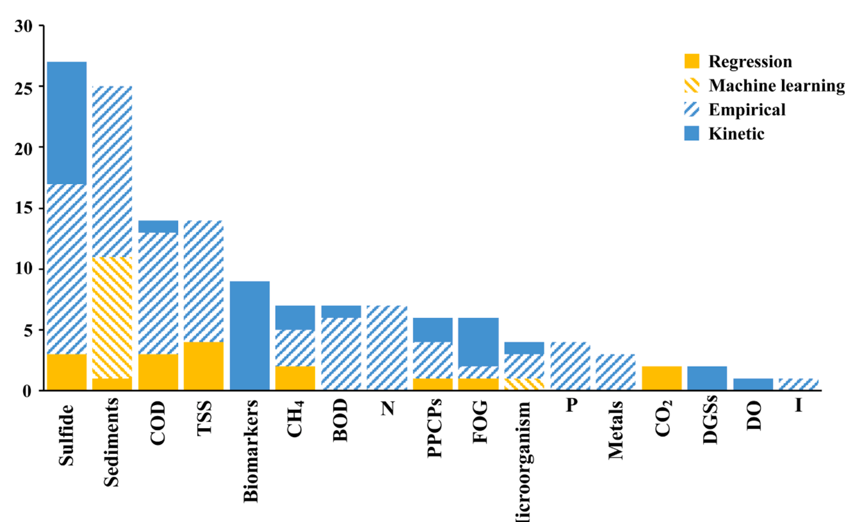

Fig. 4. Distribution of model types associated with different water quality parameters.

Table 1
Properties of the models used in the reviewed papers.

WQ parameter	Model type	Modelled process	Principal model input (s) (types)	Principal model output(s)	Model purpose	Reference(s)
sulfide	regression	production	sewer structures, season, wastewater characteristics	H_2S emission hotspots	understand the impact factors of H_2S emission	(Zuo et al., 2019)
			chemical dosage	sulfide concentration	control sulfide by chemical dosage	(Jiang et al., 2011; Jiang et al., 2010)
	empirical	production	COD concentration, temperature, pipe size, chemical dosage	sulfide production rate	predict sulfide production	(Alani et al., 2014; Marleni et al., 2015b)
			water management practices	sulfide concentration	understand the impact of water consumption on sulfide production	(Sun et al., 2015)
		mass transfer	air velocity and turbulence	sulfide concentration	improve understanding of sulfide production	(Matias et al., 2018)
			hydraulic characteristics	sulfide concentration	understand the impact of hydraulic characteristics on sulfide emission	(Carrera et al., 2017; Matos et al., 2019; Teuber et al., 2019)
		production	chemical dosage	sulfide concentration	control sulfide by chemical dosing	(Ganigue et al., 2018; Liu et al., 2013; 2016a, Sharma et al., 2014; 2013, 2012, Vollertsen et al., 2011)
	kinetic	production	COD concentration, biofilm depth	sulfide production rate, concentration	improve understanding of sulfide production	(Rudelle et al., 2012; Rudelle et al., 2013; Sun et al., 2018; Zan et al., 2019)
		mass transfer	waterfall height and fluid velocity	sulfide concentration	improve understanding of sulfide production	(Jung et al., 2017)
		production	chemical dosage	sulfide concentration	control sulfide by chemical dosing	(Abdikheibari et al., 2016; Jiang et al., 2013; Kiilerich et al., 2018; Rathnayake et al., 2019)
sediments	regression	deposition	pipe size, slope	sediment depth	predict sediment deposition	(Al-Ani and Al-Obaidi, 2019)
	machine learning (ANNs)	Deposition	pipe size, slope	blockage location	predict sediment deposition	(Bailey et al., 2016)
		transport and deposition	sediment size, sediment concentration, deposit thickness, pipe size	Froude number (which can be used for design to avoid deposit)	predict sediment transport	(Ebtehaj and Bonakdari 2014a; b, 2016; Ebtehaj et al., 2016; Najafzadeh et al., 2017; Roushangar and Ghasempour 2017; Safari, 2019; Safari and Mehr, 2018)
				critical velocity	predict critical velocity	(Mohtar et al., 2018)
	empirical	deposition	flow velocity, sediment size, sediment concentration	sediment depth	predict sediment deposition	(Campisano et al., 2019; Ota and Perrusquia 2013; Song et al., 2018)
			water management practice	sediment depth	predict sediment deposition	(Murali et al., 2019)
			pipe size, slope	blockage location	predict sediment deposition	(Baker, 2016)
		transport and deposition	TSS concentration of inflows	sediment load	predict sediment load	(Hannouche et al., 2014; Mouri and Oki 2010; Rossi et al., 2013; Seco et al., 2018; Seco et al., 2014)
			temperature, water viscosity, rainfall	sediment load, transport and mobility parameters	improve understanding of sediment transport	(Rodriguez et al., 2010; Safari et al., 2017; Shrestha et al., 2013)
		H_2S and CH_4 generation	flow velocity	H_2S and CH_4 emission	understand how the H_2S and CH_4 are generated from sediments	(Liu et al., 2016b)
COD	regression	transport	rainfall depth, rainfall intensity, CSO volume	COD concentration	predict COD concentration in the overflows of the sewers	(Brzezinska et al., 2018)
			rainfall depth, rainfall intensity	COD concentration	understand correlations between turbidity and COD	(Metadier and Bertrand-Krajewski, 2011, 2012)
	empirical	transport	hydrologic parameters, network characteristics	COD concentration	improve understanding of COD transport	(De Keyser et al. 2010; Freni et al., 2010b; Guo et al., 2019; Pablo Rodriguez et al., 2013; Torres-Matallana et al., 2018; Verdaguer et al., 2014)
			water management practice	COD concentration	understand the impact of water consumption on COD concentration	(Marleni et al., 2015a)
			sizes and slopes of interceptors, tank operation	COD concentration	control overflow pollution by operation	(Chen et al., 2019; Freni et al., 2010a; Langeveld et al., 2013)
	kinetic	hydrolysis	hydrologic parameters, network characteristics	COD concentration	improve understanding of COD hydrolysis	(Maruejouls et al., 2014)
TSS	regression	transport	rainfall depth, rainfall intensity, CSO volume	TSS concentration	predict TSS concentration in the overflows of the sewers	(Brzezinska et al., 2018; Gamerith et al., 2011)
			rainfall depth, rainfall intensity	TSS concentration	understand correlations between turbidity and TSS	(Metadier and Bertrand-Krajewski, 2011, 2012)
	empirical	transport		TSS concentration		(Cook et al., 2018)

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Table 1 (*continued*)

WQ parameter	Model type	Modelled process	Principal model input (s) (types)	Principal model output(s)	Model purpose	Reference(s)
			hydrologic parameters, network characteristics		predict TSS concentration in the overflows of the sewers	
			hydrologic parameters, network characteristics	TSS concentration	improve understanding of TSS transport	(Dembele et al., 2011; Freni et al., 2010b; Ledergerber et al., 2019; Mannina and Viviani 2010; Pablo Rodriguez et al. 2013; Verdaguer et al., 2014; Zhang et al., 2016b)
			hydrologic parameters, network characteristics	TSS concentration	understand contribution of different sources to TSS	(Pongmala et al., 2015)
			tank operation	TSS concentration	control overflow pollution by operation	(Freni et al., 2010a)
biomarkers	kinetic	degradation	temperature, biofilm area, pH, hydraulic retention time	biomarker concentration, degradation rate	understand the stability of biomarkers	(Banks et al., 2018; Gao et al., 2019; Gao et al., 2018; Li et al., 2018; McCall et al., 2017; Senta et al., 2014; Thai et al., 2014)
		biotransformation and Sorption	biofilm area, TSS concentration, hydraulic retention time	biomarker concentration	understand the impact of variables on biotransformation and sorption process	(Plosz et al., 2013; Ramin et al., 2017)
CH_4	regression	production	chemical dosage	CH_4 concentration	control CH_4 by chemical dosage	(Jiang et al., 2011; Jiang et al., 2010)
	empirical	production	surface area to volume ratio of sewer, hydraulic retention time, wastewater temperature	CH_4 concentration	predict CH_4 production	(Chaosakul et al., 2014)
			water management practice	CH_4 concentration	understand the impact of water consumption on sulfide production	(Sun et al., 2015)
		mass transfer	hydraulic characteristics	CH_4 concentration	understand the impact of hydraulic characteristics on CH_4 emission	(Matos et al., 2019)
	kinetic	production	COD concentration	CH_4 production rate	improve understanding of CH_4 production	(Sun et al., 2018)
			chemical dosage	CH_4 concentration	control CH_4 by chemical dosing	9Jiang et al., 2013)
BOD	empirical	transport	hydrologic parameters, network characteristics	BOD concentration	predict BOD concentration	(Cook et al., 2018)
			hydrologic parameters, network characteristics	BOD concentration	improve understanding of BOD transport	(De Keyser et al. 2010; Freni et al., 2010b; Pablo Rodriguez et al. 2013; Verdaguer et al., 2014)
			tank operation	BOD concentration	control overflow pollution by operation	(Freni et al., 2010a)
	kinetic	transport	hydrologic parameters, network characteristics	BOD concentration	predict BOD concentration	(Morales et al., 2016)
N	empirical	transport	hydrologic parameters, network characteristics	NH_4 concentration	improve understanding of NH_4 transport	(De Keyser et al. 2010; Guo et al., 2019; Torres-Matallana et al., 2018; Verdaguer et al., 2014)
			water management practice	NO_3 concentration	understand the impact on nitrate concentration	(Marleni et al., 2015a)
			sizes and slopes of interceptors, tank operation	NH_4 concentration	control overflow pollution by operation	(Chen et al., 2019; Langeveld et al., 2013)
PPCPs	regression	exfiltration	pipe size and material, road class	PPCPs exfiltration location	predict exfiltration location of wastewater based on PPCPs concentrations	(Lee et al., 2015)
	empirical	transport	flow velocity, DO concentration	PPCP concentration	understand whether the parameters are up to standard in particular areas	(Shahvi et al., 2016)
			catchment characteristics and population	PPCP concentration	predict PPCP concentration	(Bollmann et al., 2019; Rieckermann et al., 2011)
	kinetic	degradation	—	PPCP concentration	predict PPCPs concentration and degradation rate	(Coutu et al., 2016; Menzies et al., 2017)
FOG	regression	deposition	socioeconomic parameters	probability of FOG accumulation	understand the impact of variables on FOG accumulation	(Nieuwenhuis et al., 2018)
	empirical	deposition	pH	FOG deposits	understand the impact of pH on FOG deposition	(He et al., 2017)
	kinetic	deposition	pH, temperature	saponified solid	understand FOG deposition process	(Iasmin et al., 2016)

(*continued on next page*)

Table 1 (*continued*)

WQ parameter	Model type	Modelled process	Principal model input (s) (types)	Principal model output(s)	Model purpose	Reference(s)
			socioeconomic parameters, sewer flow	saponified solid	predict accumulation of FOG	(Yousefelahiyeh et al., 2017)
microorganisms	machine learning (ANNs)	intrusion	sewer system geometry, hydraulics, transport variables	E.coli concentration	predict the location of microbial intrusions	(Kim et al., 2013)
	empirical	transport	solid mass, hydrologic parameters	E.coli concentration	understand contribution of different sources to E.coli	(De Marchis et al. 2013; Pongmala et al., 2015)
	kinetic	growth process	shear stress	biofilm thickness	understand the mechanisms of biofilm growth	(Ai et al., 2016)
P	empirical	transport	hydrologic parameters, network characteristics	PO_4 concentration	improve understanding of PO_4 transport (by optimizing model structure, calibrating parameter, and sensitivity analysis)	(De Keyser et al. 2010; Guo et al., 2019; Verdaguer et al., 2014)
			hydrologic parameters, network characteristics	Phosphorus concentration	understand contribution of different sources to phosphorus	(Beenen et al., 2011)
metals	empirical	intrusion	network characteristics	pollutant concentration	predict illicit intrusion location	(Banik et al., 2017; Sambito et al., 2020)
		transport	spatio-temporal changes	TiO_2 concentration	understand the spatio-temporal impact on TiO_2 transport	(Kim et al., 2019)
CO_2	regression	emission	construction and operational activities	CO_2 emission	predict CO_2 emission	(Kyung et al., 2017; Zhang et al., 2016a)
toilet trash	kinetic	disintegration	turbulence intensity, solid characteristic	disintegration rate	predict the disintegration rate	(Eren and Karadagli 2012; Roni et al., 2019)
DO	kinetic	transport	hydrologic parameters, network characteristics	DO concentration	predict DO concentration	(Morales et al., 2016)
I	empirical	degradation	hydrologic parameters, network characteristics	adsorbable organic iodine concentration	understand source distribution of iodinated substances	(Knodel et al., 2011)

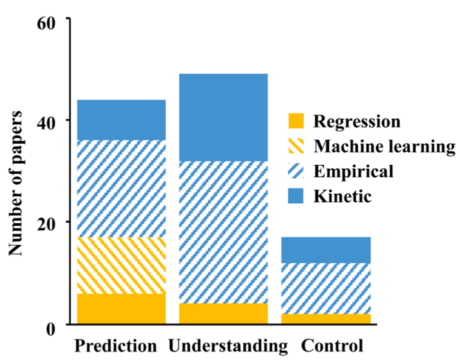

Fig. 5. Distribution of model types across different modeling purposes.

as the controlling purpose, as system control is the primary aim in these studies (Liu et al., 2016a).While models are developed for different purposes, they are ultimately (directly or indirectly) utilized to enable effective SN design, management or operations (Gamerith et al., 2011; Vollertsen et al., 2011; Ebtehaj et al., 2016).

As shown in Fig. 5, papers focusing on understanding dominate the other two categories, while papers that consider control are represented least. This is expected, as system control is often built on the prediction and understanding of the water quality parameters being considered (Sharma et al., 2014). The distribution of model types across these model purposes varies significantly, suggesting that the choice of model type is heavily influenced by model purpose. As expected, empirical and kinetic models are frequently used to enhance process understanding and to enable system control. This is because these two model types are not developed on data specific to a particular situation, but rely on (at least partly) the underlying physics and chemistry. This makes such models more transparent (i.e. ‘white-box’), as opposed to data-driven models, which are often referred to as ‘black-box’ models. Therefore, the applicability of empirical and kinetic models can be extended beyond the dataset on which they are originally tested, thereby enabling their wider adoption. As observed from Fig. 5, empirical models have been employed more frequently than kinetic models for all modelling purposes. This is because the dynamic biochemical behaviours of many water quality parameters can be significantly affected by environmental conditions (e.g., flow velocities, Teuber et al., 2019). Hence it is necessary to account for such environmental factors in an explicit manner with the aid of empirical models (Verdaguer et al., 2014). In other words, the empirical models explicitly involve the environmental factors in their model structures, but the kinetic models account for the environmental influence in an implicit manner, often using decay coefficients. Consequently, the former are more widely used compared to the latter. For prediction, the number of regression and machine learning models is significantly larger compared to those developed to enable understanding and control, as shown in Fig. 5.

Fig. 6 presents the distribution of the model types with different purposes across various water quality parameters. As shown in this figure, when the model purposes considered are process understanding or control, the empirical or kinetic model type is frequently selected for all water quality parameters. If prediction is the main purpose, regression and machine learning model types can also be used (Fig. 6), with the selection depending on the specific parameters being considered, as well as data availability (details given in the next sub-section).

Table 1 outlines the detailed purposes for different water quality models. As shown in this table, models for sulfide and COD were used for different purposes, such as concentration predictions, sewer quality and corrosion controls, as well as an understanding of the impacts of different external conditions (e.g., pH, COD and the reduced water consumption) on these two quality parameters (Marleni et al., 2015a; Sun et al., 2018). For sediments, critical velocity or sediment transport was often predicted using models (e.g., Mohtar et al., 2018), aimed at controlling pipe deposits in an effective manner (e.g., Song et al., 2018). Empirical and kinetic models were developed to understand the

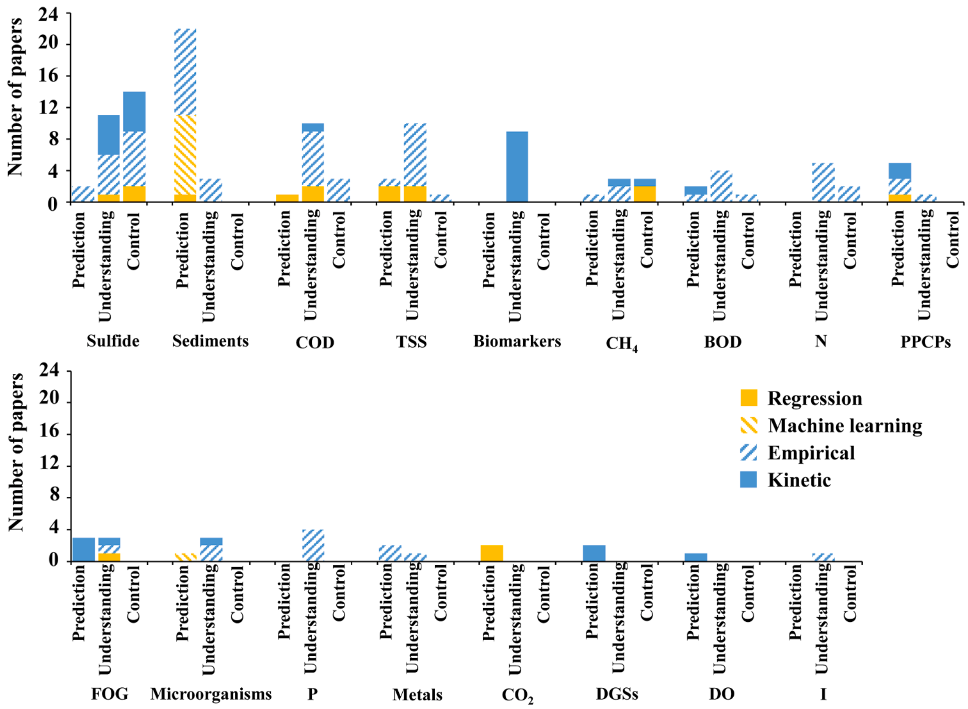

Fig. 6. Distributions of model types with different model purposes for each water quality type.

interactions between sediments and gas emission (e.g., H_2S and CH_4, e.g., Liu et al., 2016b). All the studies in the reviewed papers regarding biomarkers or microorganisms focused on revealing their degradation or growth processes, as shown in Table 2 (Thai et al., 2014; Ai et al., 2016). For PPCPs, FOG, TSS, BOD, their concentrations within SNs or in their overflows were predicted and the utility of the controlling strategies (e.g., mineralization, pump operations, changing of pH, retention tanks) assessed with the aid of models (Maruejouls et al., 2014; Nieuwenhuis et al., 2018). The descriptions of the model purposes for other quality parameters are detailed in Table 1.

In summary, the results in this section show the following: (i) the majority of the models are developed to predict and understand the behaviour of water quality parameters in SNs, with a relatively small number of models used for control, (ii) a strong correlation exits between modelling purpose and type, where purpose often determines model type (e.g., the model purpose of understanding leads to the use of an empirical or kinetic model), and (iii) regression and machine learning models are developed for the prediction of various water quality parameter values in cases where appropriate data are available; empirical and kinetic models are often used to uncover the complex biochemical processes of quality parameters such as biomarkers, microorganisms and phosphorous.

3.4. Data types used for modeling

Fig. 7 shows that the distribution of types of data used are classified into three main categories, namely experimental, field samples and continuous. Experimental data are often generated in the laboratory based on the components of water quality being considered (Safari, 2019), field sampled data are collected manually from real sewer pipes (Bollmann et al., 2019), and continuous data samples are collected from online sensors with a high time resolution (Kiilerich et al., 2018). As can be seen from Fig. 7, most of the data used for water quality model development in the reviewed papers are either experimental or taken from field samples with relatively low time resolutions. This is likley because current sensor technologies are not sufficiently well developed to provide reliable high frequency long-term online measurements for some complex quality parameters (e.g., microorganisms) (Zheng et al., 2018). It should be noted that some modeling studies used mixed data sources, where field samples were used for complex water quality parameters (e.g., COD, sulfide concentrations), and continuous data samples were used for the covariates (e.g., hydraulic and hydrologic parameters) of the quality parameters being considered (e.g., Liu et al., 2016b, Brzezinska et al., 2018, Ganigue et al., 2018). In this review, the types of data used are classified based on the water quality parameters being modeled, rather than their covariates, to enable clear interpretation.

Fig. 7 shows that empirical models, kinetic models and regression models have been developed using all three data sources, as these models can use various lengths and resolutions of data, provided that data on all requisite variables are available (Banks et al., 2018; Gao et al., 2018). It can also be seen that machine learning models (only ANNs are used, as mentioned previously) have been primarily developed using experimental data, which is likely because machine learning models often require longer data records / more data samples for their development, which can be experimentally generated more easily and cheaply. Fig. 8 presents the distribution of the data types used for model development across different water quality parameters. The figure shows that experimental data have been generated for modeling a wide range of water quality parameters. This is because many water quality models are often designed under laboratory conditions in order to understand their utility in a well-controlled environment, thereby improving understanding on their underlying processes prior to their applications to real sewer systems with field sampled data (Li et al., 2018). For example, Thai et al. (2014) designed laboratory experiments to generate data for developing an improved understanding of the degradation kinetics of various drug biomarkers, followed by the development of kinetic models to simulate the behaviour of drug biomarkers within real SNs (McCall et al., 2017) using manually collected field samples.

However, for PPCPs, CO_2 and DO, field sampled data have been used directly for model development. This might be the preferred approach because models for these water quality parameters are mainly used for prediction or control (see Fig. 7), i.e., there is less focus on process

Table 2
Case study scales and the model performance.

WQ parameter	Model type	Case study size (Total length or area of SNs)	Prediction accuracy*	Reference
Sulfide	Empirical	9.93 km (a rising main sewer)	R^2= 0.99	(Ganigue et al., 2018)
Sediments	Regression	10.5 km	R^2= 0.896	(Al-Ani and Al-Obaidi 2019)
	Empirical	2.2 km	NSE= 0.78	(Seco et al., 2018)
		1244.7 km	R^2= 0.69	(Mouri and Oki 2010)
		0.85 km^2	NSE= 0.67	(Rodriguez et al., 2010)
COD	Regression	45 km^2	R^2= 0.80	(Brzezinska et al., 2018)
TSS	Regression	45km^2	R^2= 0.79	(Brzezinska et al., 2018)
		0.45 km^2	R^2= 0.87	(Gamerith et al., 2011)
	Empirical	2.45 km^2	*NSE*= 0.85	(Dembele et al., 2011)
		80 km^2	*NSE*= 0.22	(Ledergerber et al., 2019)
		150 km^2	NSE= 0.46	(Pablo Rodriguez et al. 2013)
Biomarkers	Kinetic	1.05 (a single pipe)	R^2= 0.56	(Gao et al., 2018)
		1.05 (a single pipe)	R^2= 0.66	(Li et al., 2018)
CH_4	Empirical	3 km (a rising main)	R^2= 0.41	(Chaosakul et al., 2014)
BOD	Empirical	150 km^2	NSE= 0.43	(Pablo Rodriguez et al. 2013)
	Kinetic	3.16 km^2	NSE= 0.97	(Morales et al., 2016)
PPCPs	Regression	470 km	R^2= 0.80	(Lee et al., 2015)
Microorganisms	Empirical	6.33 km^2	NSE= 0.62	(De Marchis et al. 2013)
		7.51 km	NSE= 0.30	(Pongmala et al., 2015)

* The averaged metric value is presented when multiple values are reported in the paper.

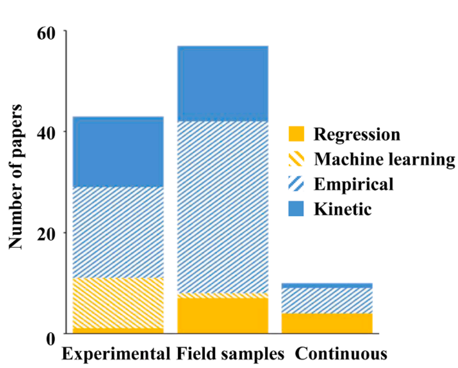

Fig. 7. Data sources available for model development.

understanding (e.g., Shahvi et al., 2016) . It is interesting to note that attempts have been made to continuously monitor H_2S (a type of sulfide, Kiilerich et al. 2018), COD (Torres-Matallana et al., 2018), TSS (Gamerith et al., 2011) and NH_4 (a type of *N*, Torres-Matallana et al. 2018) concentrations using sensors over the past few years.

From results in this section, it can be deduced that: (i) well-planned and conducted lab-scale experiments can provide useful data, especially when the goal is to improve the understanding of underlying processes of the complex water quality parameters, (ii) data from manual or automatic grab sampling can provide valuable information for specific modeling purposes at particular locations, for which grab sampling data have been widely used so far, as shown in Figs. 7 and 8, (iii) the collection of water quality data is often laborious and costly, and hence it is necessary to consider the trade-offs between the selection of model type and the effort required for acquiring the spatial and temporal data needed for model development and calibration, and (iv) while continuous online monitoring has been used for a small number of water quality parameters (e.g., H_2S and COD), its use is limited due to the high cost associated with the purchasing, installation and operation of the required sensors. However, this data type has significant future potential, not only for water quality modeling (data-driven models), but also for the development of various warning systems and new prediction approaches via data assimilation, as well as for enabling improved SN operation, asset management and planning (Zheng et al., 2018).

3.5. *Case study types that water quality models have been applied to*

As shown in Fig. 9, the number of water quality models that have been applied to real case studies is larger than that applied to laboratory problems. Fig. 9 also shows that kinetic models have been applied relatively evenly to both real and laboratory case studies, but that empirical models are more likely to be developed for real problems. among the data-driven models, regression models have been applied primarily to real case studies, with few applications to laboratory case studies, while the opposite is true for machine learning models (ANNs).

Laboratory based case studies have been used for many water quality parameters (except PPCPs, CO_2 and DO) before their applications to real problems, as shown in Fig.10. This matches well with the observations made in Fig. 8, where experimental data are shown to be widely used for water quality model development. Fig. 10 shows that models have been applied to real SNs over the past 10 years for all water quality parameters except DGSs. This implies that applications of water quality models in real SNs have been an important focus in recent years, in addition to the experimental analysis that is often used to understand their reaction mechanisms.

In summary, results in this section imply that (i) water quality models have already been frequently applied to real SNs, irrespective of model type, which is likely to lead to further developments in this area, (ii) the experience gained from models applied to laboratory based case studies under well-controlled conditions is useful for the application of such models to real problems, as highlighted in Li et al. (2018), implying that modeling quality parameters (especially for complex or newly emerged pollutants) with the aid of laboratory case studies is still an indispensable part to enable successful modeling for real SNs.

3.6. *Degree to which model performance has been evaluated*

Fig. 11 summarizes the availability of performance evaluations using an independent dataset for the different water quality model types. Although model performance was reported for the majority of studies, this was not the case for a significant number of papers (60). This is mainly because insufficient data were available to enable the evaluation of model performance. Interestingly, the performance of all ANN models was evaluated using an independent data set, likely because a large proportion of ANN models were developed with abundant laboratory data and because independent validation is common practice in the development of ANN models due to their propensity of overfitting (Wu et al., 2014; Humphrey et al., 2017). In contrast, for regression, empirical and kinetic model types, only just under half of the studies considered have carried out model performance evaluations using independent data sets, as shown in Fig. 11.

Fig. 12 shows the model evaluation status associated with each water

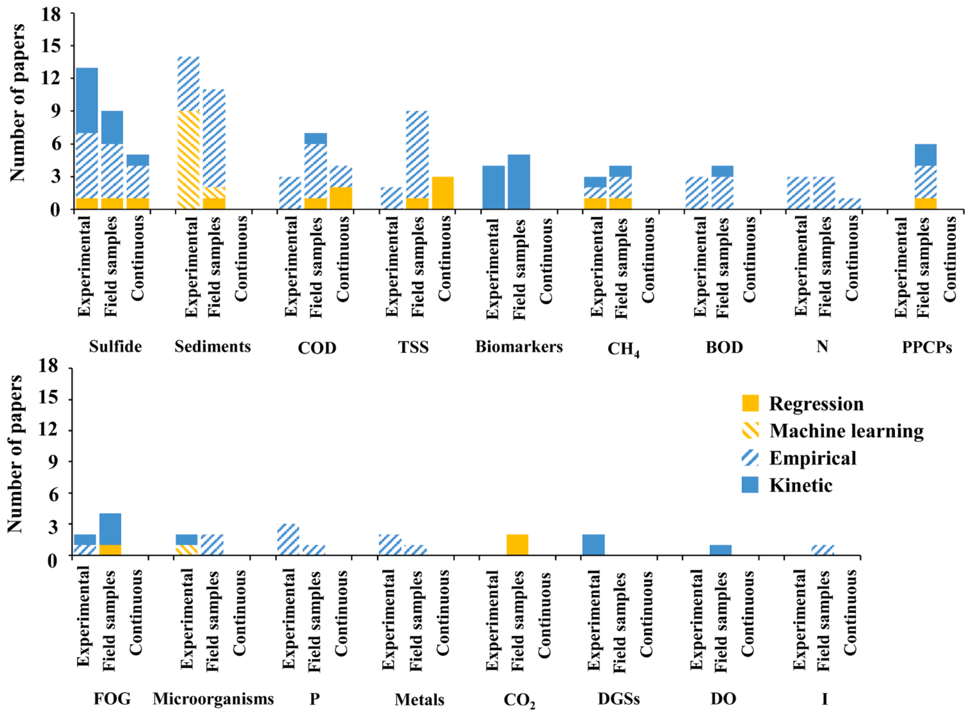

Fig. 8. Data sources for modeling of different water quality parameters.

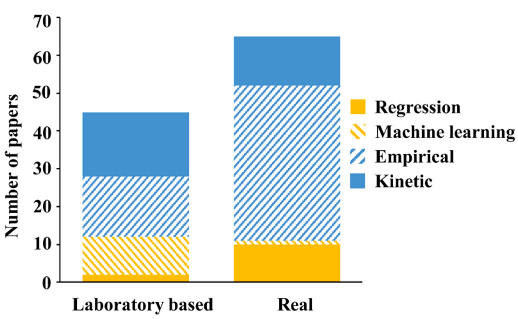

Fig. 9. Types of case studies used for model applications.

quality parameter and model type. As can be seen, for the majority of the water quality parameters, the performance of the developed models has been evaluated for some applications but not for others. The exception is models for microorganisms, for which the performance of all models has been evaluated and models for P (empirical models), metals (empirical models), CO_2 (regression models), DO (kinetic models) and I (empirical models), for which no performance evaluation was performed. In the instances where model performance was evaluated, this was generally done using observations obtained with the aid of closed circuit television (CCTV, Baker, 2016), visual inspection (Yousefelahiyeh et al., 2017) or *in-situ* measured data (Chen et al., 2019).

Table 2 shows the model accuracies for the applications where performance evaluation has been explicitly reported in terms of performance metrics R^2 and Nash-Sutcliffe efficiency coefficient (NSE). This is because these two metrics have been widely used in the reviewed papers with reported model accuracies (in about 70% of the papers with reported model accuracies). Furthermore, these two metrics are dimensionless and hence can be used to enable comparison across different quality parameters. It was observed from Table 2 that the scales of the real case studies were significantly different, with the largest SNs being 1244.7 km in length (Mouri and Oki, 2010) and the smallest SNs being 1.05 km in length (a single pipe, Gao et al., 2018). It was noted that the relatively simple and common parameters, such as sediments, COD, TSS and BOD, tended to be considered in rather larger real SNs, compared to the more complex parameters, such as biomarkers and microorganisms, as outlined in Table 2.

It can also be observed that the majority of the model applications with reported model accuracy had a relatively low level of performance, with R^2 or NSE less 0.8. In relative terms, biomarkers, CH_4 and microorganisms tended to have a lower level of model accuracy, which is due to their greater level of complexity in the processes affecting these parameters. As shown in Table 2, higher levels of model performance (R^2 or NSE greater than 0.9) were generally associated with good data availability, as was the case for empirical models for H_2S (a type of sulfide), where continuously monitored data were available (Ganigue et al., 2018), or for smaller SNs, such as the kinetic model applied to a real SN with an area of 3.16 km^2 (Morales et al., 2016). Therefore, it was concluded that models that were for relatively simple parameters, developed with a sufficient amount of data, or applied to small system scales can have overall satisfactory performances in accuracy.

3.7. Time and spatial resolutions of the model developments

among the 110 reviewed papers, 21 studies have explicitly mentioned the time resolution of the models used, with results presented in Table 3. As shown in this table, the majority of these studies use empirical and kinetic models, with only two regression models developed to understand the variations of the COD and TSS in the SNs with a time resolution of 2 min. A range of different water quality parameters were modeled with different time resolutions, including sediment, sulfide, COD and TSS (simple parameters) as well as FOG, biomarkers, PPCPs, metals, BOD and DGSs (complex parameters). It can be observed from Table 3 that, for the same quality parameters, the models with the understanding purpose had an overall higher temporal resolution compared to those developed for the control purpose. This was mainly because high time-resolution simulations can facilitate the process understanding of the water quality parameters in the SNs (often range from seconds to a few minutes as shown Kim et al. (2019)), but the control actions were often taken in a relatively low temporal resolution (often more than 15 min as shown in Ganigue et al. (2018)). However, it was

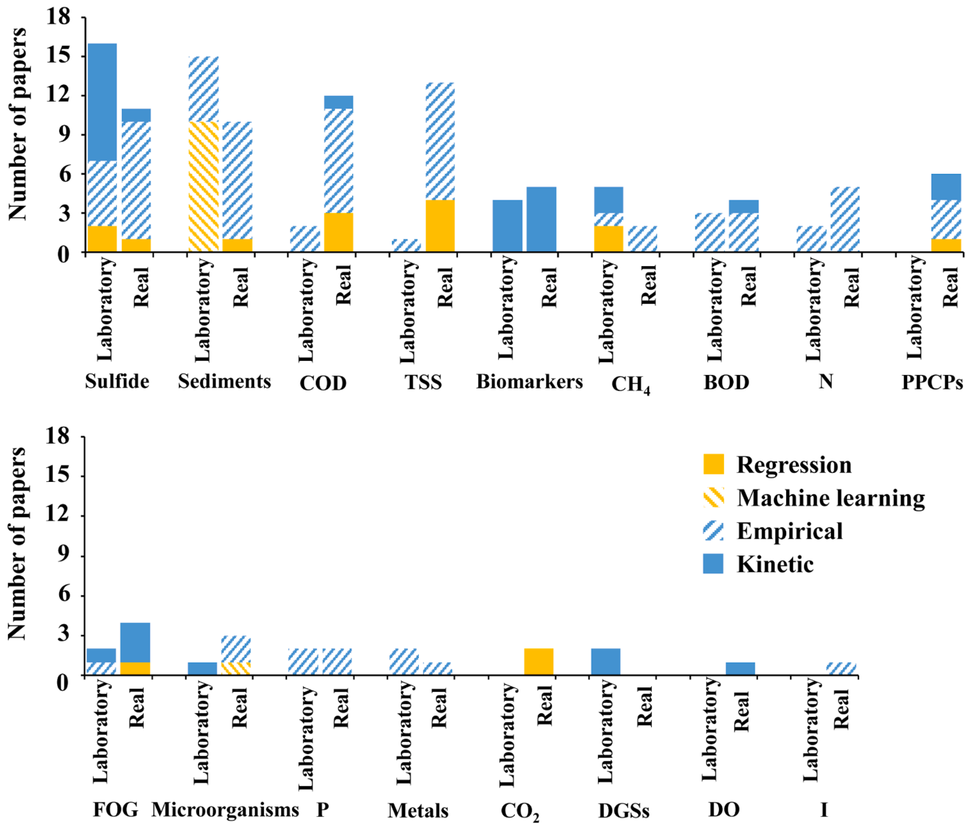

Fig. 10. Types of case studies used for model applications for different water quality parameters.

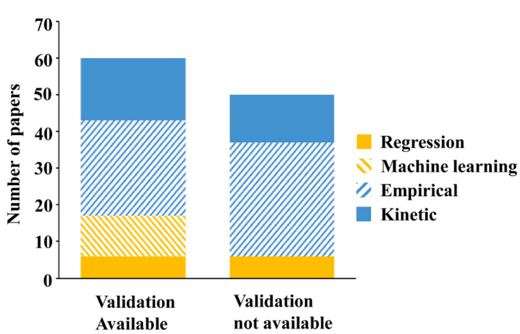

Fig. 11. Consideration of independent model performance evaluation for different model types, where 'available' and 'Not available' indicates the model accuracy validated by independent dataset is and is not given respectively.

also noted that for the same quality parameter (e.g., COD) and with the same purpose (improve the understanding), the model time resolution can be significantly varied from 1 min (Torres-Matallana et al., 2018) to 1 h (Pablo Rodriguez et al., 2013). Similar observations can be made for other water quality parameters such as sediments (the prediction purpose) and sulfide.

Table 3 also shows the performances of models that have been explicitly reported in literature, mainly using the metric of R^2 and NSE. As shown in this table, the models with a relatively high time resolution were often calibrated using experimental and continuous data sources, and hence their simulation accuracies were improved compared to the low time-resolution models that were often calibrated by data from grab samples. It is noted that none of the reviewed papers have explicitly stated the spatial resolution of their models. This is because once the empirical and kinetic models have been calibrated using the observations, the models can be applied at any given spatial resolution.

4. Current issues

Section 3 shows that significant efforts have been made over the past ten years to develop various models in order to simulate water quality parameters within SNs. However, the critical analysis of the current status of the literature has also highlighted some potential issues in relation to these models, as summarized in Fig. 13. As shown in this figure, these issues can be divided into three main categories: water quality parameters (as reflected in Section 3.2), model applications (Sections 3.3, 3.5 and 3.6), and data availability (Section 3.4).

While various models have been developed for a range of water quality parameters within SNs (Section 3.2), model applications to relatively complex quality parameters are sparse. As outlined in Fig. 4, the modeling of sulfide and sediments within SNs was addressed in 27 and 25 papers, respectively, but very few models have been developed for relatively complex parameters, such as microorganisms, *P*, DO and I over the past 10 years. This can be attributed to the corresponding complex processes involved which are not easy to capture, as well as the lack of ground-truth data at an adequate spatiotemporal resolution, which may hamper further progress in simulating these complex quality parameters. More specifically, although experiments have been designed to reveal the reaction processes of complex water quality parameters, it is still necessary to replicate and reproduce results from these existing experimental studies. In other words, it is essential to continue collecting data from real SNs to provide additional evidence on the utility of existing models for these complex quality parameters.

In recent years, in addition to many common parameters, such as sediments, H_2S and COD, some complex and newly emerged pollutants, such as biomarkers and PPCPs, have been increasingly the subject of modeling studies. However, this is still not widespread, as there are many other water quality parameters in SNs that have not been yet considered, even though their presence can significantly affect the safety and operation of such networks. For example, other types of widely used

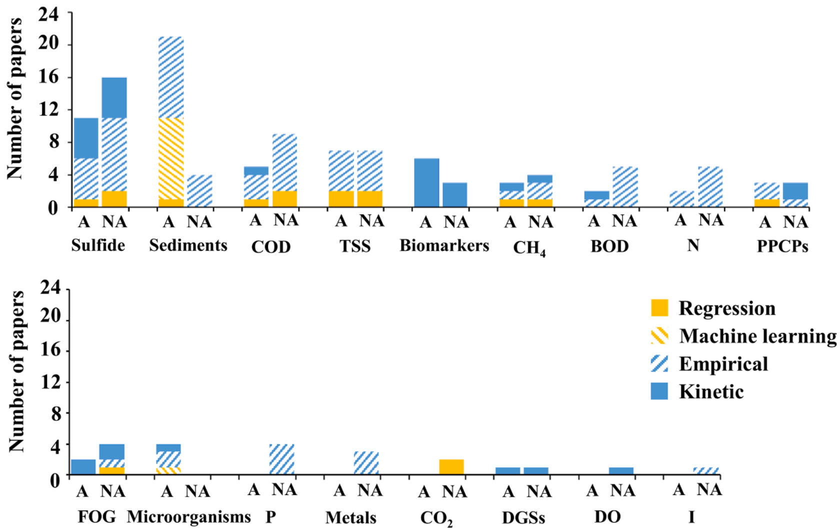

Fig. 12. Model performance evaluations for different water quality parameters, where '*A*' and 'NA' indicate the model accuracy validated by independent dataset is, and is not, available, respectively.

Table 3
Time resolutions of the developed models.

WQ parameter	Model type	Purpose	Time resolution of the model setup	Data sources for model calibration	Performance	References
Sediments	Empirical	Understanding	5 s	Grab sample	NSE= 054~0.83	(Shrestha et al., 2013)
		Prediction	1 s	Experimental	R^2= 0.899	(Song et al., 2018
			1 h	Grab sample	R^2= 0.69	(Mouri and Oki, 2010)
			10 min	Grab sample	—	(Rossi et al., 2013)
			20 s	Grab sample	NSE= 0.78	(Seco et al., 2018)
Sulfide	Empirical	Understanding	1 min / 5 min	Grab sample	—	(Matias et al., 2018)
			10 s	Experimental	—	(Teuber et al., 2019)
		Prediction	5 min	Experimental	—	(Marleni et al., 2015b)
		Control	15 min	Continuous	R^2= 0.99	(Ganigue et al., 2018)
FOG	Kinetic	Prediction	5 min	Grab sample	—	(Yousefelahiyeh et al., 2017)
Biomarkers	Kinetic	Understanding	20 s	Grab sample	—	(McCall et al., 2017)
PPCPs	Empirical	Prediction	1 s	Grab sample	—	(Rieckermann et al., 2011)
Metals	Empirical	Understanding	1 s	Grab sample	—	(Kim et al., 2019)
		Prediction	30 s	Experimental	—	(Banik et al., 2017)
COD,TSS	Regression	Understanding	2min	Continuous	—	(Metadier and Bertrand-Krajewski., 2011)
			2 min	Continuous	—	(Metadier and Bertrand-Krajewski, 2012)
COD,BOD,	Empirical	Understanding	15 min	Experimental	—	(De Keyser et al. 2010)
COD,TSS, BOD	Empirical	Understanding	1 h	Grab sample	NSE= 0.43/0.46	(Pablo Rodriguez et al. 2013)
COD	Empirical	Understanding	1 min	Continuous	NSE= 0.78~0.80	(Torres-Matallana et al., 2018)
		Control	30 min	Continuous	—	(Langeveld et al., 2013)
DGSs	Kinetic	Prediction	11.57 s	Experimental	—	(Roni et al., 2019)

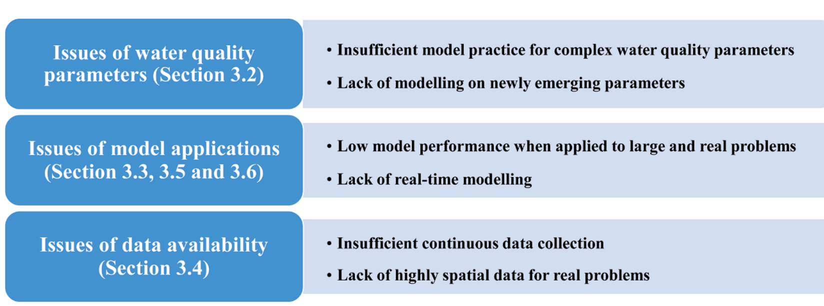

Fig. 13. Identified issues of the current water quality modelling practice within sewer networks.

personal care products, such as antimicrobials, sunscreen agents and preservatives, can be toxic on aquatic organisms when discharged from sewer networks. Their impact on receiving water bodies and adverse effects on human beings can be significant (Wang and Wang, 2016; Grassi et al., 2013). While some modeling concepts have been developed to quantify the emission of these personal care products in sewer networks, such as the discharge to raw water through CSOs (e.g., O'Brien et al., 2017; McCall et al., 2017; Pouzol et al., 2020), their dynamic behaviors in SNs are not yet comprehensively simulated. Another type of emerging contaminant are endocrine disruptor compounds (EDCs) that can have negative impacts on both wildlife and humans, even at very low concentrations (Balest et al., 2008; Falade et al., 2018). However, EDCs have not yet been sufficiently modeled in SNs. In more recent years, microplastics have been increasingly recognized as harmful anthropogenic contaminants that cause physical and chemical damage to exposed aquatic organisms and accordingly represent threats to human health (Chua et al., 2014; Cole et al., 2015; Ziajahromi et al., 2017). Future modeling practice should consider such new contaminant types to enable SNs to be managed, as also highlighted in Rodrigues et al. (2018).

The second category of issues is related to model applications (Fig. 13). The performance of models applied to large and real problems is overall moderate, or even low, as outlined in Table 2. This is likely due to the high level of complexity of the reaction process of the quality parameters being considered in larger SNs (Pongmala et al., 2015), as well as the low spatial resolution of the data used for model development (Ledergerber et al., 2019). It is also observed that almost all SN quality models developed so far are offline models. While such models are generally sufficient for scenario analysis (Pongmala et al., 2015), system design or long-term management (Gamerith et al., 2011; Pablo Rodriguez et al. 2013), they are not well suited to real-time modelling of SN water quality parameters, which is therefore an area that should be considered in the near future due to the growing need for real-time system management (Creaco et al., 2019).

The third common problem associated with current water quality modeling practice within SNs is the lack of data (Fig. 13), including insufficient continuous data collection for specific locations, as well as a lack of the spatial data needed for model development for practical applications. This is likely to be the main reason that the performance of many models has either not been evaluated (see Fig. 12) or is unsatisfactory (Table 3) (these models have not been well calibrated using a sufficient amount of data based on the evidence provided in Section 3). This data scarcity is mainly caused by: (i) the difficulties/challenges involved in measuring complex water quality parameters (microorganisms, metals, PPCPs and biomarkers), especially in a real-time fashion (De Marchis et al. 2013; Cong et al., 2015), and (ii) the low sensor density within real SNs due to the high cost of sensor purchase, installation and maintenance (Ishihara, 2017).

5. Future directions

Based on the current state of water quality modeling efforts in SNs (Section 3) and the identified issues within their applications (Section 4), it can be concluded that efforts should be made to improve water quality modeling of SNs by intensively collecting data and improving the understanding of underlying physical processes of quality parameters. It is also important to build true collaboration between practitioners and academia in order to ensure a wider adoption of good modeling methods and guidelines, as well as their applications in real SN studies. Since data shortage and reliability is currently a significant bottleneck, the development of corresponding uncertainty analysis techniques is encouraged to overcome issues in the short term, i.e. whilst waiting for data from more widespread deployment and new sensors to be collected.

In addition to these efforts, three important/key future directions for research in this field are identified as follows:

(a) Develop novel approaches to collect water quality data of different types at improved quantity, quality and accuracy and at lower cost. As reflected by the review, a bottleneck within the SN water quality modeling is the lack of data, which consequently results in a number of issues, including insufficient model practice for complex or newly emerging parameters (Fig. 4), low model performance when dealing with real problems (Table 2) and inability of real-time management (Fig. 13). Therefore, it can be derived that collecting data at improved quantity, quality and accuracy and at lower cost is critical to underpin the future development of improved water quality models in sewer networks. This includes the following research sub-directions.

Ø Development of new and improved water quality sensors. The primary objective is to develop sensors that are able to acquire data that are currently difficult or virtually impossible to collect, or that are currently too expensive to collect, as this requires specialist equipment, expertise and service. This is an important way to enable the model developments for complex water quality parameters as well as newly emerging parameters, which are identified issues within the SN water quality modeling domain as shown in Fig. 13. One example of this is the data collection on the biofilm parameter where microorganisms associated with the biofilm need to be manually taken from the sewer pipe, followed by the measurement with the aid of a microscope (Ai et al., 2016). Another example is the detection of organism or virus that causes SARS-CoV-2, which at this point in time requires at least 24 h for the sample to be taken to the laboratory and analyzed using the reverse transcription quantitative polymerase chain reaction (RT-qPCR) techniques (Medema et al., 2020). The entire process is time consuming as well as requires specialist equipment and expertise to enable accurate measurements. The additional objective is to collect wide-ranging water quality data with improved frequency, accuracy and reliability and at lower cost. This is required for a range of applications in SNs, but especially the development of real-time water quality models, which is a growing need in recent years (Fig. 13) to support more efficient and automated system operation, control and management (e.g., warning of illicit discharges, Creaco et al. 2019).

Ø Develop novel approaches to identify optimal spatial and temporal data resolutions for various water quality parameters. As shown in Fig. 7, the majority of data used for model developments are taken either from laboratory or from limited field samples. This is mainly because the in-situ continuous data collection is often expensive, especially for complex parameters (e.g., PPCPs). To solve this issue, one promising way is to identify optimal spatial and temporal data resolutions for various water quality parameters, in addition to developments of new and improved water quality sensors as previously stated. Typically, collecting data at a resolution that is higher than required would result in unnecessarily high sensor costs and model development effort. However, a data resolution that is too low would not be able to represent well the temporal and spatial variations of interest, and would hence lead to models with reduced performance (Geli et al., 2009; Ouattara et al., 2013). For example, the temporal resolution of data used for modeling microorganisms can be significantly lower than that for a common parameter such as TSS. This is because the evolution dynamics of microorganisms can be appreciably slower than that of TSS. To achieve optimal data resolution, it is critical to understand the comprehensive biochemical processes of water quality parameters in SNs. This is especially the case for the more complex parameters (e.g. biomarkers, PPCPs and microorganisms) and some newly emerged pollutants (e.g. EDCs). However, for quality parameters with relatively slow evolution processes, it may not be necessary to develop high temporal or spatial resolution models to simulate their reaction behaviors within SNs.

(b) Develop improved water quality models for SNs by developing hybrid models. There is a growing need to improve the prediction accuracy and reliability of various water quality models, as many have shown low to moderate prediction accuracy levels, especially for complex water quality parameters and complex reaction mechanisms (e.g., P) or for large real SNs (see Table 2). In this context, the development of hybrid models is proposed as a possible future research direction (Maier et al., 2010; Mount et al., 2016). For example, hybrid models could be useful in cases where the degree of understanding of the different sub-processes to be modeled is variable, in which case empirical or kinetic models could be used to account for the processes that are well-understood, with data-driven models used to model the residual relationship between model inputs and outputs. A similar approach could be used to account for cases where there is variability in the availability of data, including a mixture of grab samples for some parameters possessing relatively low reaction dynamics (e.g., PPCPs and microorganisms) and continuous data for parameters with relatively quick reaction rates in the SNs (e.g., TSS). Hybrid models seem appealing especially in cases where the underlying physical, chemical and biological process are so complex that the process-driven modeling of respective water quality parameters would be impractical or virtually impossible, even with improved quantity and quality of observed data. In these cases, empirical or kinetic models could be used to represent the main underlying processes of interest, with data-driven models used to explain the rest of prediction variance, i.e. the underlying patterns that may not be immediately obvious, often due to lack of relevant knowledge. This way hybrid models can lead to the ultimate goal of generating new knowledge and insights, thus advancing the field of water quality modeling in sewer networks. While hybrid models have rarely been used in the SN water quality modeling area so far, their success in other domains, such as hydrology (Hunter et al., 2018), can demonstrate their great ability in making best use of existing data and physical knowledge for model developments.

(c) Improve model transferability between different sewer networks and applications. Within this comprehensive review, it was found that almost all water quality models are developed for specific applications. Therefore, their calibrated model parameters, as well as the reported model performances, are conditioned on specific data collection approaches, data availabilities and even operational scenarios. Therefore, the reported model performances are not actually robust (Table 2). More importantly, these models often need to be substantially modified or even completely rebuilt when applying to different SNs or applications, which requires significant effort. The low transferability of these SN water quality models is a problem that has been ignored for a long time period, which has significantly hampered their practical use. Therefore, an important future direction in this field is to develop models that can transcend specific case studies, thereby improving model transferability so as to enable their wider uptake for practical applications. To achieve this goal, it may be necessary to investigate the scalability of the developed models across different problems and operational scenarios.

6. Conclusions

This review discusses progress with regard to water quality model development in urban sewer networks (SNs) over the past 10 years. Based on the outcomes of this review, we can summarize the main conclusions as follows:

(i) Four main types of models that simulate water quality parameters in SNs are identified. These are regression models, machine learning models, empirical models and kinetic models. It is found that the use of empirical and kinetic models dominates over the use of data-driven models for many quality parameters (Figs. 3 and 4). This is because the empirical and kinetic models typically have greater model transparency and generalization ability across different problems and operational scenarios, making them more attractive for practical applications. In addition, the development of data-driven models (regression and machine learning models) generally also requires a larger amount of data, which can be difficult and expensive to obtain for real SNs. Furthermore, in the past, academic research has favoured the development of empirical or kinetic models over data-driven ones, but this trend is changing now and both types of models have a role to play in future water quality modeling of sewer networks.

(ii) The main applications of water quality models are identified as prediction, process understanding and control of sewer networks (Table 1). It is observed that empirical and kinetic models are primarily used for understanding and control purposes, whereas regression and machine learning models are mainly used for prediction (Figs. 5 and 6). This can be attributed to the fact that empirical and kinetic models possess higher model transparency, and hence do not need to adjust their model structures when faced with system variations caused by control or operation actions. In contrast, data-driven (regression and machine learning) models tend to be good at forecasting due to their ability to effectively learn patterns in the observed data.

(iii) Experimental data generated in the laboratory and limited field grab samples are the two main data sources for water quality model development, with limited attempts made to collect online continuous data for the same purpose (Figs. 7 and 8). This trend results in the wider uptake of empirical or kinetic models due to the fact that they require relatively less data for their development compared with data-driven models. Therefore, the increasing availability of continuous (i.e. sensor) data is likely to lead to wider developments of data-driven and hybrid models, where for the latter methods data-driven and empirical or kinetic models are used jointly.

(iv) Many water quality models have been developed and applied to real SNs (Figs. 9 and 10), but the evaluation of their performances needs further improvements. For example, the performances of these models have often not been evaluated using an independent, validation data set (Figs. 11 and 12). In addition, some models have shown low to moderate prediction accuracy levels, especially for complex water quality parameters and complex reaction mechanisms (e.g., P) or for large real SNs (Table 2). It is believed that this is, at least partly, due to the fact that the underlying reaction processes of the quality parameters within real, large SNs are not well understood, as well as the lack of data available for model calibration.

(v) A number of other important issues that exist within SN water quality modeling are identified. These include insufficient consideration of complex and newly emerged quality parameters, lack of real-time modeling and insufficient observed data (Fig. 13).

To address the issues mentioned above, three specific future research directions are suggested: (a) development of novel approaches to collect water quality data of different type, improved quantity, quality and accuracy and at lower cost; (b) development of improved water quality models, especially hybrid type models that involve empirical, kinetic and data-driven methods working together to overcome various limitations that exist currently in both approaches; this approach will also enable the modeling of complex water quality processes and phenomena that are currently virtually impossible to model; (c) improvement of model transferability between different sewer networks and applications, i.e. development of more general and robust water quality models that can be transferred between different case studies and applications without the need to make substantial model updates. It is highlighted here that advancing the modeling of water quality in SNs needs greater efforts involving multidisciplinary research and sharing of best practices across different quality parameters, both between various research groups but especially between practitioners and academia.

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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