Modeling hydraulics and water quality in distribution networks: a review of existing mathematical techniques and software

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Chapter Outline

10.1 Introduction

Water distribution networks (WDN) are composed of vertical and linear components. Vertical components include pumping stations and storage facilities, whereas linear components include transmission mains and distributions system pipelines [1]. These components depend on the source water (e.g., surface, groundwater, and seawater) and topography [2,3]. Typically, linear components are more expensive with a value ranging from 60% to 80% of the total cost of the water supply systems [4]. WDNs are complex systems consisting of a considerable number of components such as series of pipes, reservoirs, valves, and pumps, causing a nonlinear intrinsic problem with implicit constraints [5,6].

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The hydraulics of water flowing through distribution pipes are affected by topography (e.g., slope), pressure, flow velocity, and pipe characteristics such as diameter, length, and pipe materials [7]. The hydraulics also affects the water quality. Water age and stagnation are primarily controlled by WDN design and system demands. This means water age can vary significantly in a WDN. Increased water age can raise water temperature, which can cause reactions to occur faster and go further. Water age can exacerbate water quality problems, such as disinfection by-products (DBPs) formation, pipe corrosion, nitrification, and microbial growth and regrowth [8].

The design of WDNs involves the estimation and prediction of hydraulics and water quality for ensuring water supply with adequate quantity and quality. This requires mathematical modeling. WDNs can be modeled using optimization techniques such as classical methods: linear, nonlinear, and dynamic optimization. In particular, a nondeterministic polynomial-time hard (NP-hard) problem [9−11] can be used for computation, which is highly time consuming and complex to be solved. Regarding complex nature of these systems, conventional design methods such as classical optimization models cannot aggregate all desired aspects of modeling; and a proactive approach should be considered to have a comprehensive plan for maintenance, rehabilitation, and/or replacement in the future [12]. Also, continuous visual inspection of a mostly buried system of water distribution is not possible due to its significant costs. Therefore methods are required to predict the performance of WDNs. In addition, computer software and tools, such as EPANET and WaterCAD, are used extensively to assist the design and analysis of water distribution systems.

This chapter aimed to review the recent advancements in mathematical methods, tools, and software applied in modeling WDNs and elaborates the applications, strengths, and limitations of available mathematical models, methods, and software. The findings can facilitate researchers and industrial practitioners in strengthening their knowledge of performance assessment of WDNs with respect to hydraulics and water quality.

10.2 Methodology

To conduct this study, an extensive literature review was carried out to understand various mathematical and hydraulic modeling techniques in water quality and distribution network. A systematic approach was adopted to comprehensively review challenges of modeling, prediction methods, tools, and software, while interaction between hydraulics and water quality is also investigated. Fig. 10.1 shows the main components of the overall review process. Published literature includes peer-reviewed journal articles, conference proceedings, book chapters, and reports compiled by various governmental and nongovernmental bodies to acquire the relevant information.

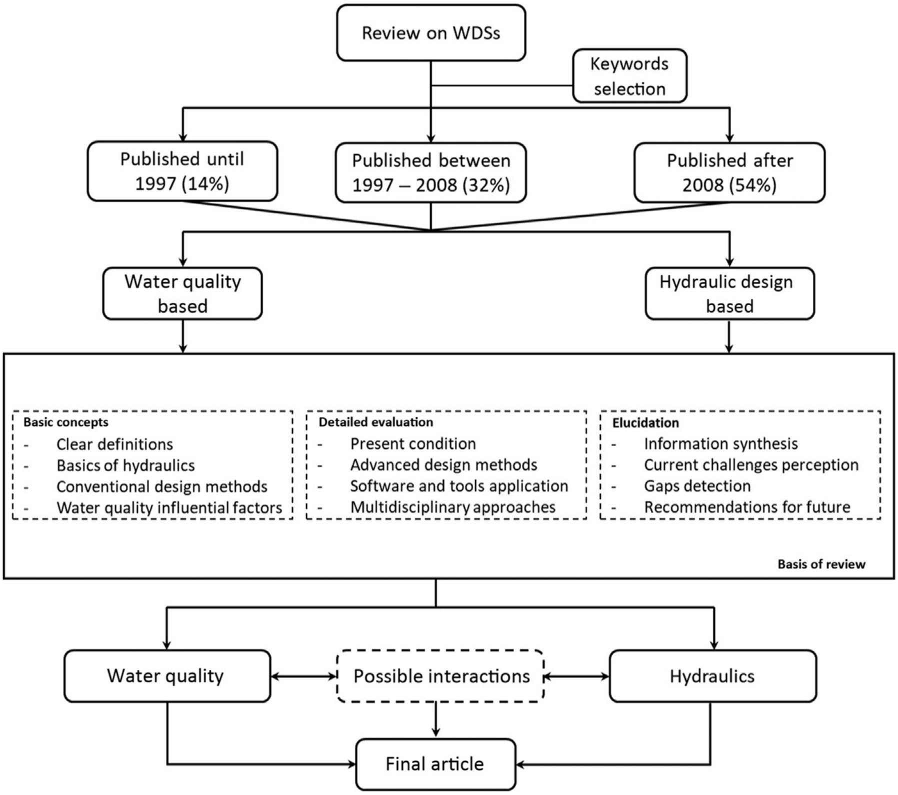

Figure 10.1 Methodological framework.

The articles were selected from a reference pool consisting of more than 83 research articles. Out of them, 54% of the literatures were collected post-2008, 32% of literatures were derived between 1997 and 2008, and the remaining 14% literatures were gathered pre-1997. To focus on up-to-date and high-quality information, recently published articles were prioritized. The articles were gathered from different notable journals such as Science of Total Environment, Journal of Water Management, Journal of Water Resources Management, Journal of American Water Works Association, Journal of Hydraulic Engineering, Water Research Journal, Urban Water Journal, Water, Environmental Modelling & Software, Computer and Mathematics with Application, Water Resources Research, and Journal of Environmental Engineering. The web-based search engines that were used to search articles include Google Scholar, Science direct, electronic library of the University of British Columbia, and Compendex Engineering Village. The keywords used for this search comprise "water quality," "hydraulic modeling," "water distribution networks/systems," "predictive models," "software and tools," "drinking water," "soft computing methods," "data-driven models," and "optimization."

10.3 Hydraulics in water distribution network

10.3.1 Fundamental of hydraulics

The study of hydraulics enables us to calculate flows, velocities, head losses, and water levels in a WDN. A typical WDN in water supply system is shown in Fig. 10.2. The raw water collected from sources (lake, river, or wells) is pumped to a water treatment system. The treated water is pumped to a WDN that is composed of pipes having several nodes at which different pipes join.

In modeling hydraulics, a Chezy equation (Eq. 10.1), Manning equation (Eq. 10.2), and Hazen–Williams equation (Eq. 10.3) are used to calculate the velocity of flow in pipes. All three equations are used for a uniform flow. Flows in both WDN and sewer mains are uniform (i.e., longitudinal water velocity is same) but not permanent (flow and velocity vary with time); however, there exists a

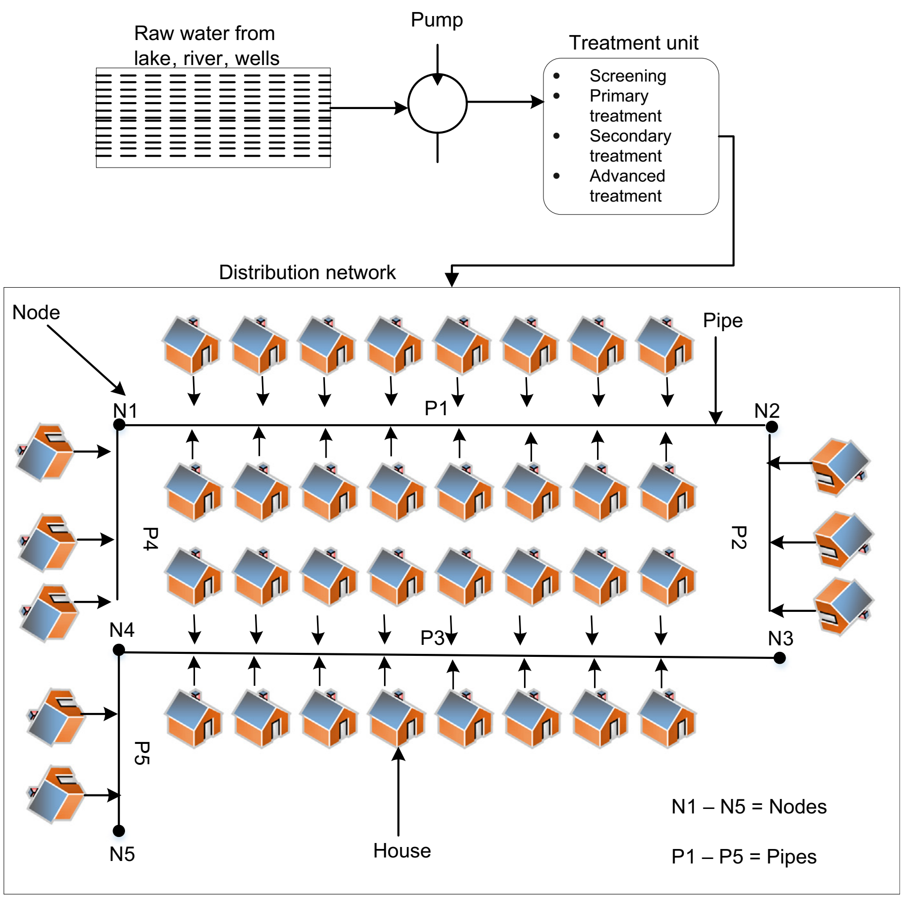

Figure 10.2 A water distribution network in water supply system.

difference in pressure. In sewer mains, water pressure is usually maintained at 1 atm, while in WDN, pressure is maintained higher than 1 atm. For the former case, Eqs. (10.1) and (10.2) are used, while latter case uses Eq. (10.3) for the velocity computation [7]:

$$V = C_c(R_h \times s)^{1/2} \tag{10.1}$$

$$V = \frac{{R_h}^{2/3} \times s^{1/2}}{n} \tag{10.2}$$

$$V = 0.849\ C_{\mathrm{HW}} \times R_h^{0.63} \times s^{0.54} \tag{10.3}$$

where V is the velocity of flow measured in m/s, C_c the Chezy's constant, R_h the hydraulic radius measured in m, s the slope of energy grade line, n the Manning's coefficient of roughness, and C_{HW} the Hazen–Williams roughness coefficient.

To calculate the head losses, Darcy–Weisbach equation is used, which is given by the following equation:

$$H_L = f \times \left(L \times V^2\right)/(d \times 2 \times g) \tag{10.4}$$

where H_L is the head losses due to pipe friction measured in m, f the friction factor, L the length of pipe measured in m, and g the acceleration due to gravity measured in m/s.

In fluid dynamics, conservation of mass, momentum, and energy are considered as governing equations. The conservation of mass states "If for an isolated system a quantity can be defined that remains precisely constant, regardless of what changes may take place within the system, the quantity is said to be absolutely conserved." The conservation of momentum states that "the sum of the forces acting on the volume of fluid equals the time rate of change of momentum" [13].

The energy conservation between two points a and b is expressed through Bernoulli equation as given in Eq. (10.5). The equation states that the difference in energy between two points is the sum of head losses. The hydraulics considered here includes only pressure energy, kinetic energy, and potential energy [7].

$$\left(\frac{Pa}{\rho g} + \frac{v2a}{2g} + ha\right) - \left(\frac{Pb}{\rho g} + \frac{v2b}{2g} + hb\right) = \text{head losses} \tag{10.5}$$

where $\left(Pa/\rho g\right)$ is the pressure energy measured in m, $\left(v2a/2g\right)$ the kinetic energy measured in m, and h the potential energy measured in m.

10.3.2 Design methods

From the computational point of view, design of WDNs shall be considered as an NP-hard problem [9–11], which is highly time consuming and complex to be solved. Regarding complex nature of these systems, conventional design methods such as classical optimization models cannot aggregate all desired aspects of modeling; and a proactive approach should be considered to have a comprehensive plan for maintenance, rehabilitation, and/or replacement in the future [12]. Also, continuous visual inspection of a mostly buried system of a WDN is not possible due to its significant costs. Several recently developed methods used for predicting the performance of WDNs in the future have been evaluated in this section.

10.3.2.1 Classical optimization

Some of the most common classical optimization techniques are as follows:

Linear programing: Linear programing is one of the most common classical optimization methods that help to find the optimum solution for a continuous problem with respect to linear objective function subject to linear constraints. It is widely used in design and operation of WDN [14]. This method is capable of determining the optimum extremely quickly and directly [15]. Samani and Mottaghi [16] used linear programing to study the optimum design of municipal WDN through an iterative procedure, which fulfills all the design constraints (i.e., pipe sizes, velocities, reservoir levels, and nodal pressures) with a minimum cost. Zangeneh and Samani [15] used mixed integer real linear programing (LP) technique that can quickly obtain information related to pipe sizes, pumps, and reservoir heights having short nodal pressure constraint equations, which can assist in design of a WDN.

Nonlinear programing: Nonlinear programing can handle WDNs of a restricted (i.e., limited) size as it contains limited number of variables and constraints. Unlike linear programing, it does not cover global optimum solution, while dealing with WDNs but works with continuous variables [14]. Zheng et al. [17] combined nonlinear programing (NLP) with differential algorithm in a looped WDN to optimize the pipe diameters for the shortest distance tree requiring less computational efforts. Al-Hemairi and Shakir [18] developed a model to optimize the operation of control valves using a nonlinear objective function that brought less pressure differences resulting in low leakage rates.

Dynamic programing: Dynamic programing is a technique that breaks down a complex problem into a sequence of multiple simple problems such that each of simpler problems is solved just once and stored in form of array or maps. In WDNs, dynamic programing is mostly suitable for pump scheduling applications [19]. Bashi-azghadi et al. [20] studied the time-dependent management strategy in a contaminated WDN using dynamic programing. The authors concluded that for small-scale decision variables, dynamic programing is superior both in terms of accuracy and computation.

10.3.2.2 Advanced optimization

In the design and evaluation of WDNs, there is an obvious trade-off between general objective functions of cost and reliability mostly used in the system design, various shapes of objective functions, and inexplicit forms of constrains.

Subsequently, there are obvious benefits in the application of advanced optimization, such as evolutionary algorithms (EAs) including compatibility with discrete problems, independence from derivatives calculation, adaptability to a wide range of objective functions, and obtaining a range of efficient solutions [10].

A considerable number of benefits can be achieved using the hydraulic simulation of WDNs such as optimization of system variables, calibration of parameters, online monitoring of the system, and management of system assets such as valves operations [21]. To this end, the application of coupled optimization and simulation models provided designers and decision-makers with capable computational tools to design and rehabilitate hydraulic systems [22−24]. Optimal design of Drinking Water Systems (DWSs) was first considered as a single objective deterministic problem solved by classic optimization methods such as linear programing [25−28] and the generalized reduced gradient technique [29]. Later on, genetic algorithm (GA) as an evolutionary optimization algorithm was used to solve the problem by Dandy et al. [30,31] for the first time.

Hitherto, a wide range of EAs has been increasingly used in the design/rehabilitation of WDNs by a considerable number of studies due to their high capacity for solving nonconvex and nonlinear optimization problems with both continuous and discrete decision variables [32−40]. In the mentioned researches a wide range of EAs has been applied on WDNs including multiobjective swarm optimization, nondominated sorting GA 2 (NSGA2), ε-NSGA2, strength Pareto EA 2, multiobjective prescreened heuristic sampling method, harmony search (HS), differential evolution (DE), and a multialgorithm genetically adaptive multiobjective. While until 2005 most of the researchers utilized a single objective optimization approach to model WDNs networks, one study [41] performed multiobjective optimization providing Pareto fronts (a trade-off curve) to select optimal solutions based on desired balance between different objective functions. They developed an uncertain methodology with less simplification and better efficiency.

Most of the researchers in this field used EPANET as a numerical solver to find the node pressure calculation and perform hydraulic simulation [9,12,41−43]. Through the application of EPANET, the flow rate of the nodes and head loss in the loops of the network are evaluated to satisfy the mass conservation as well as energy conservation principles, respectively, which are considered as two important constraints of optimization approaches. Generally, pipe size availability, minimum and maximum pressure of each node, and minimum and maximum velocity of each pipe were considered as other constraints of the problem in different studies mostly applied using penalty method and also by choosing decision variables through optimization process [5,9]. The objective function for this problem was mostly considered as minimization of a WDN construction and operational cost [5], as well as maximization of system's reliability [43] or resiliency considered by different definitions, such as probability of minimum requirement satisfaction in all nodes of the network [41], maximization of network resilience considering excess head (additional to minimum requirement), and number of reliable loops [9], and so on. Also, a wide range of decision variables such as the specification of hydraulic structures, properties of different pipes of the network, and application of rehabilitation strategies have been selected in this optimization problem.

Several research tried to apply new and/or hybrid multi-objective evolutionary algorithms (MOEAs) such as water cycle algorithm or hybrid optimization algorithm, for example, by combining HS and GA [43] or combining the high exploration (better in global search) capacity of DE with desired exploitation (better in local search) capacity of HS in a multiobjective optimization [9] to enhance the performance of optimizers. In addition, to evaluate the performance of the optimization algorithms, several metrics have been considered in optimization of WDNs including generational distance [44], diversity (D), hypervolume [23,44], and coverage set [45] in different researches [9]. These performance metrics measure the diversity and/or convergence abilities of MOEAs.

It is also necessary to mention that there are two types of uncertainty sources—one relates to the lack of information about different parts of the network and the other relates to fluctuations in different parameters, such as water demand. The latter may be dealing with consideration of probability density functions such as Gaussian distribution for related parameters [41]. It is also possible to consider various sources of uncertainty in WDNs including consumer demands, the water level at tanks, the flow rate in pipes, and so on [42]. There are three different general methods to take uncertainties into account including fuzzy logic or possibility theory, probability theory, and consideration of bounds for uncertain variables [41]. To take the effects of uncertainties into account, different methods of sampling such as Latin hypercube sampling as well as a Monte Carlo simulation process mimicking, for example, demand pattern were used in combination with optimization process in the field of WDN design [41,42].

10.3.3 Prediction models

To predict pipe failures (mechanical failures) in a WDN to enhance the mechanical reliability of the system, it is necessary to establish a relation between the number of pipe bursts and system properties. This purpose requires capable predictive tools to provide designers and decision-makers with an idea about possible future pipe bursts in the network [5,46,47]. A new paradigm has been formed in the design of WDNs in recent years shifting from traditional linear or nonlinear optimization approaches into the application of soft computing methods such as metaheuristic/evolutionary optimization algorithm, and data-driven models (DDMs). Due to the considerable potential of soft computing methods, a large number of studies have been performed in the field of WDN design by the application of DDMs and coupled optimization and numerical models.

10.3.3.1 Data-driven models

A variety of factors affect the pipe burst rate including pipeline age, environmental factors such as frost depth, construction quality, and service conditions such as flow pressure in the network [5,46,48]. As mentioned, an appropriate relation between these variables and pipe failure/pipe burst rate (annual number of pipe failure in its unit length) in the network can be obtained using numerical models. The variety of numerical methods including deterministic regression models, multivariate models, probabilistic methods, and DDMs have been developed to predict the number of pipe bursts in WDNs [46]. While there are considerable discrepancies in results acquired by statistical and conventional regression methods, DDMs are capable methods considering a large number of parameters involved in a highly complex system such as a WDN [9,47].

As mentioned, the other soft computing methods widely used in the design and rehabilitation of WDNs are different types of DDMs such as Gaussian process regression (GPR), support vector regression (SVR), evolutionary polynomial regression (EPR), and artificial neural network (ANN). All these methods estimate the future condition of a WDN based on the records of data such as previous pipe bursts collected during an acceptable period.

Assuming a dataset like $D = \{(x_i, y_i)|i = 1, 2, ..., n\}$ in which x_i and y_i represent input and target variables, respectively, a GPR will predict related outputs of new input variables (x_i^*). In the Gaussian process, used in this approach, target values (outputs) are determined using a summation of a regression function ($f(x)$) and a noise value (ε) [46].

Also, SVR is a supervised machine-learning approach that can be used to estimate a function or predict a phenomenon. In this method, coefficients of a linear/nonlinear function should be determined while minimizing the approximation error between observed data and calculated outputs of the model. To minimize loss function (error) in this method, Lagrange duality theorems in combination with a classic optimization method such as quadratic programing or EAs may be utilized for linear or nonlinear problems, respectively [46].

The other DDM that can be used to predict the required output based on available records of pipe failures is ANN. Input, output, and hidden layers consisting of different neurons form the main structure of an ANN. Related weighting coefficients defining relations between neurons of different layers should be determined using nonlinear mapping minimizing the difference between observed data and estimated outputs. To this end, a set of data shall be divided into three different subsets of training, validation, and test for the determination of weights and verification of the model [46].

Moreover, EPR is a type of data-driven methods in which a general formula is defined, and its constant parameters are determined using multiobjective EAs concerning the minimization of the number of explanatory variables and maximization of model fit to observed data. The general form of a polynomial EPR model is as follows:

$$Y = \sum_{j=1}^{m} F\left(X, f(X), a_j\right) + a_0$$

where Y is the desired output, a_j the different coefficients of the assumed polynomial, X the matrix of explanatory variables, f a predetermined function (e.g., an exponential function), m the maximum number of polynomial terms to achieve an appropriate trade-off between complexity and fit, and a_0 is an unknown constant. Coefficients of the abovementioned polynomial can be determined using a method like least square [5].

Several other models such as different regression models including linear, exponential, Poisson generalized linear, and logistic generalized linear model as well as hybrid ANN and adaptive neuro-fuzzy inference systems have been considered to predict pipe failures in a WDN [47,49].

10.3.3.2 Fuzzy concept

Fuzzy logic was proposed by Zadeh in 1965 [50]. The concept assists to solve real-life problems that deal with vague, subjective, and imprecise information [51]. Fuzzy set theory is rigorously used in civil and water resource engineering. Sadiq et al. [52] applied fuzzy sets to predict failures in WDN. Islam et al. [53] used a fuzzy-based methodology to detect and diagnose leaks in WDN by considering uncertainties in distribution network's pipe roughness, nodal demands, and water reservoir levels. Zhang et al. [54] implemented fuzzy technique that detects pipe bursts in WDNs based on characteristic values and similarity analysis. Moosavian and Lence [55] used fuzzy set theory for the analysis of WDN with epistemic uncertainty.

10.3.4 Challenges of modeling and prediction methods

Water quality modeling is considered an important tool for utility managers to design WDNs and analyze various processes involved in distribution network. The development of water quality model (WQM) dates back to the mid-1990s, which was mechanistic in nature. These models (i.e., also known as first-generation models) were focused to understand biofilms in water and wastewater treatment processes [56]. One of the challenges observed in these models was its complexity in expanding to the entire distribution network [57]. In addition, models involved complex equations and had no link with hydraulic parameters making them difficult to implement in real WDNs. The second-generation models came into existence at the beginning of the 20th century. Although models developed during this generation contained simplified equations and had connection with hydraulic, model's inability to identify the precise concentration of contaminants and oversimplification of advective transportation of contaminants in WDN were some notable challenges. Hence, the overall challenge of water quality modeling is to meet the simulation results precision and necessary resources that help to solve computational problems [58].

The challenges of predictive modeling are as follows:

- Predictive models can be very complex, requiring data for many different parameters, which can be time consuming.
- Predictive models can consist of many uncertainties. These uncertainties can reduce the accuracy of the prediction.

10.4 Water quality modeling for water distribution network

Safe drinking water is a fundamental human right. In drinking water management, safe water refers to water quality, which also reflects the presence of contaminants in drinking water. These contaminants in drinking water are physical, chemical, and microbial. The chemical and microbial contaminants pose threat to human health. Thus water is required to treat adequately to ensure safety. Water supplied to consumers through interconnected infrastructure through water supply system [59]. The most critical components of water supply system are WDNs. The performance of WDNs in the context of human health protection is generally assessed by the quality of water being delivered to consumers [60]. Due to the pressure of growing population, climate change, and aged infrastructure, contaminants discharge is influencing water quality far more than ever. Governments are taking actions to fulfill the needs of stakeholders and control the presence of contaminants by regularly monitoring the water quality [61]. The transport and assimilation of pollutants at various locations in distribution systems are a matter of concern for water supply managers and municipal authorities. Water quality sampling monitoring is a time-consuming process. Furthermore, there is a cost to perform the sampling and monitoring and to track spatial and temporal variations in pollutants. This has led to the development of WQMs. A model offers a mathematical description of the attributes of system under study and expresses some representation of the attributes of the system. A model refers to a "simplified representation of a system (or process or theory) intended to enhance our ability to understand, predict, and possibly control the behavior of the system" [62]. Hence, model is a reflection of system's reality, which involves the understanding of system's components.

10.4.1 Historical development

The development of WQM is a challenging task because of the complex and nonlinear nature of the water treatment processes. The information of water flows and contaminant loading are the basic requirements to develop a WQM. Collecting data of contaminants is considered as a crucial step while developing a WQM, which is translated into mathematical simulations of the system by considering all underlying processes [62]. Selecting the right data/information and maintaining the data accuracy facilitates in developing a reliable model. The development of WQMs began in the mid-1990s. All models developed at that time were mechanistic. The models developed initially were complex as they considered a list of variables to run. The modifications and improvements in WQMs continued, some major development in modeling in the 1990s are as follows:

1. *Development of commercial modeling tool:* The first version of EPANET was released in 1993. The EPANET becomes very popular for conducting various water quality and hydraulic modeling studies. EPANET can model networks including all WDN components physically drawn in the user interface. Development of this software has facilitated

designers and researchers to conduct study on the water quality and hydraulic assessment in distribution system. Until now, EPANET is one of the commonly used software due to its compatibility with other software and it is simple to use and requires no license to use.

2. *Modeling of disinfectant and DBPs*: Due to growing concerns of microbial contamination, the water utilities applied disinfection to inactive the pathogens from the drinking water. However, the concentration of disinfectants varies within the WDN. In 1994 a mass transfer−based model for predicting chlorine decay was introduced. This model facilitated in estimating the presence of residual disinfectants in different locations of WDN. Furthermore, the DBPs were in spotlight from the 1970s, which were typically formed considering the reaction of natural organic matter in drinking water and residual disinfectant concentration. Chlorine was the most commonly applied disinfectant and it led to the formation of THMs (trihalomethanes) and HAAs (haloacetic acids) in drinking water. Several kinetic and empirical models were developed for THMs and HAAs in the context of WDNs during that time.
3. *Modeling water quality in tanks and reservoirs*: USEPA conducted several studies to assess the impacts of water storage tanks on the water quality supplied to WDNs. Several models and mechanisms related to water age and water mixing in storage tanks were observed. The model includes both mathematical and physical models.

In the 20th century the development of second-generation models was observed, which couples WQMs with hydraulic models. This was considered as a huge success in the water sector [63]. Furthermore, the 20th century identified some new areas of emphasis for application and research, for example, water security issues, water age modeling, real-time operational modeling, and modeling the behaviors of transformation and processes.

10.4.2 Water quality processes modeling

Broadly, two types of processes occur in WDNs—bulk and walled. The bulk processes involve the reaction of chemical in bulk flow of water and are affected by the quality of treated water flowing into the network [64]. Walled process refers to the interaction of water with pipe material or with the material accumulated at the pipe surface. Hence, they are influenced by the condition and material of pipe. To assess the quality of water in WDNs the understanding of these processes and their influence on water quality parameters are critical.

The underlying concept of the WQM is the mass balance principle [65]. Mass balance principle states that the mass entering a system must, through mass conservation, equal to mass leaving the system or accumulating within the system.

Mathematically, the mass balance for a system is described by the following equation:

$$\text{Output} = \text{Input} \pm \text{accumulation} \tag{10.6}$$

To apply mass balance concept the WDN is divided into segments or compartments, and the water quality constituents entering the system must be equal to the sum of constituents leaving and accumulating within the system over a given time period. For simulating water quality, time is taken as discrete intervals and water flows are considered constant for each of those time periods. Then, mass input and output for a substance are observed for each time interval within each segment of the system. The WQMs in general are developed considering a complete and instantaneously mixing. Once the mixing is done, the substance undergoes both advection and dispersion transport [63]. Advection transports refer to the horizontal movement by flowing water, whereas dispersive transport refers to the molecular diffusion of substance and results from concentration gradient. In general, the constituent concentrations inside pipe wall are function of constituent transport and are explained by using mass balance models [66]. With deeper understanding of the water quality reactions and considering some assumptions, the simple model used to highlight the advection and transportation mechanism is given in the following equation:

$$\frac{dC}{dt} = -U\frac{dC}{dx} + kC \tag{10.7}$$

where C is the reactant concentration at time t; u, mean flow velocity; and kC, rate of reaction. Furthermore, considering only reaction aspect, it is assumed that the rate of chemical reactions is known to be affected by constituent concentrations and it decreases as the concentrations decrease. This type of reaction follows first-order kinetics, which assumes that the rate of a reaction is proportional to the concentration of constituent. Mathematical expression of simplified reaction is shown in the following equation:

$$\frac{dC}{dt} = -kC_0 \tag{10.8}$$

where C is the reactant concentration; t the elapsed time; k the reaction rate constant (dependent on reaction); and C_0 the initial concentrations. Generally, natural systems follow first-order kinetics, while the second-order kinetics are preferred to study the system where rate of reaction is proportional to the square of the concentration of single constituent. For example, the decomposition of liquid bleach (NaOCl), in basic solution, follows a second-order process [67].

Mathematically, second-order kinetics is expressed in the following equation:

$$\frac{dC}{dt} = -kC_0^2 \tag{10.9}$$

In addition, the issue of corrosion is addressed though the development of solubility models. Metal pipes are integral component of a WDN and corrosion of these pipes can cause excessive levels of lead, copper, or iron in water. The presence of these metals in water poses potential health risks and must be monitored regularly. The knowledge of solubility models provides guidance for water treatment adjustments such as changes in pH levels, dissolved inorganic carbon, and orthophosphate to reduce mineral levels in water. A solubility model is specific to each metal compound and is determined through field and laboratory experiments to obtain a solubility constant. The value of solubility constant along with water chemistry data is used to predict the concentration variations under different conditions of pH and inorganic carbon [68]. For example, corrosion of lead pipes is a major concern for human health and can be controlled by altering the water chemistry and minimizing lead solubility in water. The major parameters contributing to the lead solubility are pH, carbonate, and orthophosphate. As the pH increases over 8.0, a decrease in lead solubility can be observed and water is made safe for population use [69].

The water quality within a WDN, during supply from the outlet of the treatment plant to the consumer's tap, is affected by microbial, chemical, and physical hazards. Microorganisms enter the distribution system through a variety of ways (e.g., cross-connections, pipes breaks, open storage tanks) and grow in the form of biofilms near the end of the distribution. The formation of biofilm exhibits tolerance against the action of disinfectant and lessens the effectiveness of these chemicals. Chemical hazards include DBPs, which are formed when a disinfectant reacts with organic matter in the water. These DBPs lead to the leaching of metal pipes and formation of metal ions, thus exhibit toxic effects for human health. The most common type of physical hazard present in WDN is turbidity or the presence of sediments. These particles may clog the pipes as bacteria can adhere to these sediments and grow. For the past few decades the awareness about deterioration of water quality and regulations of water management authorities has encouraged the use of modeling approaches in water quality [61].

10.4.3 Water quality models

Water quality parameters such as oxygen, disinfectant residual, DBPs, watercolor, smell, and turbidity are investigated in water quality modeling. Chlorine residual perhaps is the most commonly studied parameter. The algorithms used to simulate chlorine decay in a distribution system are based either on steady-state or dynamic approaches. The dynamic approach is considered to be more accurate because it allows the simulation of changes in the spatial distribution of pollutants under a time-dependent demand. The dynamic models can further be classified as Eulerian- and Lagrangian-based models. In the Eulerian models, pipes are divided into equally sized segments, whereas the Lagrangian models divide pipes into variable segments.

Based on 1-D advection–diffusion, the chlorine residual model is written as shown in the following equation:

$$\frac{\partial c_{i,t}}{\partial t} + v_i \frac{\partial c_{i,t}}{\partial x} + D_x \frac{\partial^2 c_{i,t}}{\partial x^2} + R(c_{i,t}) = 0 \qquad (10.10)$$

where $c_{i,t}$ is the cross-sectional average chlorine concentration in pipe i as a function of distance x and time t; v_i the flow velocity in pipe i; t the time; D_x the diffusion coefficient in direction x; and $R(c_{i,t})$ the reaction rate as a function of concentration. Furthermore, Al-Omari and Chaudhry [70] found that in turbulent flow the diffusional effect can be neglected as shown in the following equation:

$$\frac{\partial c_{i,t}}{\partial t} = -v_i \frac{\partial c_{i,t}}{\partial x} - R(c_{i,t}) \tag{10.11}$$

where $R(c_{i,t})$ describes the intensity of bulk and wall reactions occurring between chlorine and other substances in a pipe, which also accounts for the major part of the total source-sink effects:

$$R(c_{i,t}) = -k_0 c_{i,t} \tag{10.12}$$

where k_0 is the first-order reaction rate, indicating that the chlorine decay rate is proportional to the chlorine concentration in the first power. The first-order reaction rate can be determined as:

$$k_0 = k_b + \frac{k_w k_f}{r_h(k_w + k_f)} \tag{10.13}$$

where k_b is the bulk decay coefficient; k_w the wall demand coefficient; k_f the mass transfer coefficient; and r_h the hydraulic radius. In practice, the values of k_w, k_b, and k_f can be obtained through field calibration; however, Musz et al. [71] reported that the availability of k_b and k_w could be a challenging issue in water quality modeling. Hence, assuming the values of those coefficients based on experience becomes a popular practice.

Rossman et al. [72] developed a 1-D advection−reaction model to predict the chlorine residual in water distribution systems by considering the radical chlorine transport and reaction at the pipe wall. This model was incorporated in the well-known water quality modeling software package EPANET. The latest version of the software package, EPANET 2, is one of the most widely used water quality modeling tools for WDNs. It enables simulation of nonreactive tracer materials, chlorine decay, DBP formulation, and water age [73]. EPANET 2 can model the dynamics of a single chemical such as chlorine residual and THM in a WDN; however, it cannot be used to simulate the interaction of different chemicals. To overcome the limitation, researchers have developed many extension models based on EPANET 2. For example, Shang et al. [74] developed the EPANET-MSX model that enables the simulation of multiple chemical species in networks by considering their reactions and the reactivity of water from different sources. Sohn et al. [75] developed a two-phase kinetic model for THM modeling. The two-phase model takes the interaction of chlorine and THM into account:

$$c_{\mathrm{THM}} = c(A(1 - \exp(-k_1 t) + B(1 - \exp(-k_2 t))) \tag{10.14}$$

where c is the chlorine concentration; k_1 and k_2 are the fast and slow chlorine decay rate constants, respectively; and A and B the fast and slow reacting components of THM, respectively.

Another limitation of EPANET 2 is that the hydraulic analysis is demand driven, which could generate unrealistic hydraulic and water quality modeling outcomes in the presence of network irregularities (e.g., temporary demand change, pipe break, and pump failure). Siew and Tanyimboh [76] also developed the EPANET-PDX to simulate hydraulic performance and water quality through a pressure-driven approach. EPANET-PDX can model the water quality of a network under both normal and pressure-deficient conditions. The logistic pressure-dependent demand function was used in the EPANET-PDX [77]:

$$Qn_i(Hn_i) = Qn_i^{\mathrm{req}} \frac{\exp(\alpha_i + \beta_i Hn_i)}{1 + \exp(\alpha_i + \beta_i Hn_i)} \tag{10.15}$$

where Qn_i is the flow at node i; Hn_i the head at node i; Qn_i^{req} the demand at node i; and α_i and β_i are parameters to be calibrated with field data. When field data are not available, α_i and β_i can be calculated using empirical equations:

$$\alpha_i = \frac{-4.595 Hn_i^{\mathrm{des}} - 6.907 Hn_i^{\mathrm{min}}}{Hn_i^{\mathrm{des}} - Hn_i^{\mathrm{min}}} \tag{10.16a}$$

$$\beta_i = \frac{11.502}{Hn_i^{\mathrm{des}} - Hn_i^{\mathrm{min}}} \tag{10.16b}$$

where Hn_i^{des} is the nodal head above which $Qn_i = Qn_i^{\mathrm{req}}$; Hn_i^{min} the nodal head below which Qn_i is zero. Seyoum et al. [78] assessed EPANET 2-MSX and EPANET 2-PDX in water quality modeling of chlorine residual, DBPs, and water age under different operating pressure. They found that both EPANET 2 extensions provided the same water quality modeling results under normal operating pressure but different results under deficient pressure. They also concluded that using the two extensions of EPANET 2 could help to obtain more accurate water quality modeling results. Although EPANET can generate relatively accurate prediction results of chlorine residual in water transmission mains, it becomes less accurate when predicting chlorine residual in secondary branch pipes ("dead ends" of a system) [79]. A dynamic 2-D convection–diffusion equation to describe the mass balance on disinfectant concentration in dead ends can be written as:

$$\frac{\partial c}{\partial t} = -\frac{\partial (v \cdot f(r) \cdot c)}{\partial x} + \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial c}{\partial r}\right) - k_{\mathrm{b}} c \tag{10.17}$$

where c is the solute concentration; x and r are the axial and radial coordinates (m), respectively; t the time (s); v the average flow velocity in the pipe (m/s); $f(r)$ the radial flow distribution parameter; D the molecular diffusivity of solute in water (m^2/s); and k_b the first-order decay constant (s^{-1}) in the bulk water.

The chlorine consumption at the pipe wall could be simulated:

$$\frac{\partial c}{\partial r} = -\frac{cW_d}{D} \tag{10.18}$$

where $r = a$, the pipe radius (m); W_d the wall demand parameter (m/s). The equation only applies to fast chlorine reaction at the wall; for pipes with significant biofilm thickness a two-layer mass transfer approach would be more suitable. The above 2-D convection−diffusion model requires intensive computation. Practitioners often reduce the model to an unsteady 1-D advection−dispersion model to preserve the dynamic behavior of solute transport:

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + E\frac{\partial^2 c}{\partial x^2} - Kc \tag{10.19}$$

where E is the effective longitudinal dispersion coefficient (m^2/s); K the overall lumped first-order decay constant (s^{-1}) that accounts for solute decay in both the bulk phase and at the pipe wall. k can be calculated using Eq. (10.9). Reducing a 2-D model into a 1-D model could bring the error caused by neglecting the combined effects of radical molecular diffusion and the parabolic flow velocity in the radial direction. It is important to determine the appropriate dispersion coefficient in the steady laminar flow based on the Taylor [80] equation:

$$E = \frac{a^2 v^2}{48D} \tag{10.20}$$

where a is the pipe radius (m); v the average flow velocity (m/s); D the molecular diffusivity (m^2/s).

Lee [81] developed a dynamic time-evolving dispersion coefficient to simulate the complex laminate flow demands in dead ends.

$$E_k(t) = E_{k-1}(t_{k-1})\left(\frac{v_k}{v_{k-1}}\right)\exp\left(-\frac{t - t_{k-1}}{t_0}\right) + E_{T_k}\left[1 - \exp\left(-\frac{t - t_{k-1}}{t_0}\right)\right] \tag{10.21}$$

where E_{k-1} is the instantaneous dispersion coefficient for pulse $(k-1)$; t_{k-1} the ending time of pulse $(k-1)$; E_{Tk} Taylor's dispersion coefficient for pulse k; and $t_0 = a^2/16D$ is a Lagrangian time scale. The time-averaged rate of dispersion during any pulse k is determined as:

$$\overline{E}_k = \frac{1}{(t_k - t_{k-1})}\int_{t_{k-1}}^{t_k} E_k(t)dt \tag{10.22}$$

Based on the dynamic time-evolving dispersion coefficient for pulsating laminar flows, Abokifa et al. [82] developed a model named WUDESIM to simulate disinfectant residuals in the dead ends of water distribution systems. Their model accounted for the combined effects of the spatial and temporal distribution of flow demands on disinfectant transport. The simulation results of WUDESIM showed better agreement with field measured concentrations than the advection-based model EPANET.

Furthermore, with the issue of DBPs occurrence in WDNs the water utilities have switched the disinfectant type from chlorine to chloramine. The chloramine decay in WDNs occurs due to chemical and microbiological reactions. Generally, WQMs have been applied and used to model the behavior of chloramines in WDNs. The model facilitates in developing a better understanding of the effect of water quality parameters on the disinfection consumption. Recently, a new WQM was proposed to estimate chloramine residual considering the chemical and microbiological factors. To develop a new approach for WQMs the chloramine decay equations were applied to EPANET-MSX and chloramine decay was assumed to be described by the sum of two first-order equations. It was suggested to use the developed model as a guide in decision making to choose the appropriate strategies to reduce monochloramine consumption and improve the disinfection process particularly to avoid nitrification [83].

10.4.4 Interaction between hydraulics and water quality

As the bulk water travels through the WDN, the water undergoes various chemical and physical transformations, resulting in an impact on water quality. Many factors have an influence on the transformations, including water demand, water flow rate, finished water quality, pipe conditions, and deposits in the distribution system. These factors are interrelated and have impacts on both water quality and hydraulic performance of the system. For example, water age is a function primarily of water demand, system operation, and system design, and a long water age may cause water quality problems. System design and operation are linked to the hydraulic performance of the system. It is a common practice to design a water distribution system that can meet future demand (e.g., 20 years or more) [8]. This would increase water age in the short term as the storage volume in the facility will be larger than the present-day demand.

The Water Industry Database indicates an average distribution system retention time of 1.3 days and a maximum retention time of 3.0 days in the United States; however, it is not uncommon to observe long water age (e.g., >300 h) in some cases [84]. As water demand and/or flow rate increases, the retention time of water in the system decreases. Water conservation, particularly the use of reclaimed water on-site, will tend to lead a longer water age. Prolonged water age could cause or worsen water quality parameters, such as the formation of DBPs, decay of disinfectant, compromising corrosion control effectiveness, and causing unpleasant taste and odor [85]. Also, longer water age can increase water temperature, increasing the rate of reactions and intensifying water quality problems, such as nitrification and microbial growth and regrowth [8]. On the other hand, some water quality issues, such as high concentrations of minerals and the rapid decay of disinfectant (or insufficient disinfection of water), will cause deposits of minerals and formation of biofilm in the distribution system. The deposits of minerals and formation of biofilm would change the configuration of pipes and joints, ultimately altering the hydraulic performance of the entire system [85].

10.5 Software and tools for modeling water distribution network

The design of water distributions is complex and time consuming. A continuous research and development have been taking place in hydraulic and water quality modeling. Many new methodologies, approaches, and algorithms have been developed to improve the performance of models and increase the model applicability considering variable conditions. Table 10.1 lists commonly used software for modeling hydraulic and water quality in WDN [63].

Water quality modeling in distribution system is showing a steady growth and maturation considering the last four decades. Several models and methods were developed and validated to evaluate the water quality performance of a WDN. In addition, several software to design and evaluate the performance of WDN. However, there is still a need for continuous field measurements to collect water quality data, which can be used to establish more WQMs and validate the previously developed models. Furthermore, the model performance in modeling software can be further improved by adding more input water quality features. There models with reliable results can be used as a benchmark for comparing the performance of WDN in terms of water quality and hydraulics.

10.6 Conclusion and recommendations

Water flowing in a WDN undergoes continuous variations in terms of hydraulics and water quality due to the interaction of water quality constituents with themselves and also with pipes. Several factors, such as pipe diameters, length, topography, pressure, and water quality status itself, affect the overall water quality. WDNs can be designed using classical and/or advanced optimization methods, which will basically show hydraulics. The variation in hydraulics can be modeled and predicted using several data-driven methods, whereas water quality can be predicted modeling water quality processes albeit they are highly dynamic. Both hydraulics and water quality modeling are performed and improved using tools and software. Many such software are commercially available. The major challenges of modeling are that the models can be very complex, requiring data for many different parameters, which can be time consuming. Also, the models can contain many uncertainties, reducing the accuracy of the models. These findings provide fundamental knowledge of WDN modeling by elaborating the applications, strengths, and limitations of available models and software. In addition, these findings can facilitate academic researchers and industrial practitioners in strengthening their knowledge of performance assessment of WDNs regarding WDN hydraulic and water quality.

Table 10.1 Commonly used water distribution network (WDN) design and modeling software.

SN	Modeling software/ tool	Quality modeling	Hydraulic modeling	Key features
1.	InfoWater	✓	✓	• A GIS-based WDN modeling software • Capabilities of performing network optimization • Geospatial analysis • Infrastructure planning and management
2.	KYPipe	✓	✓	• Ability to conduct hydraulic analysis, considering different WDN sizes • Model water distribution pipes and fire demand, and performing pump optimization • Compatible with GIS and AutoCAD
3.	H_2OMap Water	✓	✓	• GIS-based modeling platform for WDN • Ability to perform energy management, fire flow analysis, and unidirectional flushing • H_2Omap extension package "H_2Omap Water MSX" can model complex water quality reactions
4.	AFT Fathom	×	✓	• Fluid dynamic simulation software • Applied in oil and gas industry, water and wastewater system design, infrastructure management sector
5.	WaterGEMs	✓	✓	• Comprehensive WDN design software • Capable of conducting intelligent planning and optimized operations • Ability to identify water losses, manage energy use, fire flows, and real-time network simulation • Compatible with AutoCAD
6.	EPANET	✓	✓	• Most commonly used software to model WDN • Simple and easy to use, no license is required • Compatible with AutoCAD and Google earth • Extension packs are available to model water quality and multiple contaminants

(*Continued*)

Table 10.1 (Continued)

SN	Modeling software/ tool	Quality modeling	Hydraulic modeling	Key features
7.	GOODwater	×	✓	• Design software for small WDN • Ability to generate optimum cost of pipes • Cover aspects related to sustainability including sociocultural, economics, and environment
8.	Synergi Water	✓	✓	• Strong database management • Capable to perform quick and accurate analysis for large WDN • Integrated with GIS and SCADA
9.	WaterCAD	✓	✓	• Commonly used to design and model large WDN, powerful tool • Can interface with AutoCAD • Capable of assessing the WDN hydraulics and operational modeling, fire flow, criticality, and water quality analysis; and in developing flushing plans, identifying water loss, and managing energy use

GIS, Global intelligence system; *SCADA*, supervisory control and data acquisition.

The recommendations of this study are as follows:

1. Long-term field data on water quality are required to improve the existing WQMs and establish new models for several other water quality parameters.
2. The model performance in modeling software can be further improved by adding more input water quality variables in the models. These models with reliable results can be used as a benchmark for comparing the performance of WDNs in terms of water quality and hydraulics.
3. The interactions between hydraulics and water quality are studied only for limited parameters such as water age, chlorine residuals, and DBPs. Further studies are required to model the interaction among other several hydraulic and water quality parameters.
4. Hydraulics and water quality data can be used to monitor and indicate the status of water infrastructure, such as pipe condition in terms of leakage. An advanced technique such as artificial intelligence can be used to monitor hydraulics and water quality and predict pipe and water quality failure in advance for its control.

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