Challenges of Water Quality Modelling in Drinking Water Supply Systems

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Abstract
Drinking water quality (bacterial regrowth, discolouration, taste and odour) deteriorates within water distribution systems (WDS). This is governed by several factors: inlet water quality, hydraulic conditions, disinfection reagent, temperature, substrate etc. To predict drinking water quality within the WDS mathematical models can be used.
During last 30 years there has been numerous drinking water quality models developed. This paper summarizes the advantages/drawbacks of most common models and points the future challenges for drinking water quality modelling.
The first generation models has begun to appear in literature in middle of 1990`s. All of these models described in literature are based on mechanistic models of biofilms in water and wastewater treatment processes. Using these models it was possible to simulate spreading of chemical or biological contaminant in single pipe. The drawbacks of the models where too complex equation and constant schemes to adapt them to the real scale WDS, and models were not linked to hydraulic parameters of WDS.
At the beginning of 20th century the second generation models appeared. Those models are connected to hydraulic models of WDS. The equations and formulas where simplified to apply them for real scale WDS drinking water quality simulations. Although, it was a great step forward in water quality modelling, and it was possible to model the contaminant spreading into real scale WDS, the results showed that the models shows only the characteristics of the contaminant spreading but not the precise concentrations of it. The disadvantage of second generation models are that there is instantaneous and perfect mixing in junction assumed. Also the assumption that there is only advective transport of contaminant in WDS is oversimplified.
Improvements of the second generation models has been done during the last ten years, however there are still a lot of work to be done to implement them to real scale WDS modelling. The studies about the incomplete mixing have been done and advective-dispersive mass transport has been introduced into water quality modelling. However, at the given moment all of those improvements demand a huge computational resource. The main challenges of the water quality modelling are to meet the requirement of the precision of simulation results and the available computational resources.

Keywords
Drinking water, distribution network, modelling

INTRODUCTION

All around the world there are strict requirements for drinking water purification and there are special limits for microbial quality of drinking water. The limits and requirements for drinking water quality in European Union are specified in Drinking Water Directive (DWD) 98/83/EC. The limits for *Eschericia coli* (*E.coli*) is 0 cells in 100 ml of water and for heterotrophic plate count (HPC) is 100 colony forming units (CFU)/ml after water cultivation on media for 3 days at 22ºC (EUC 1998). Since the DWD requirements allows small concentration of microorganisms in drinking water and the water purification processes in water treatment facilities are effective and high quality, safe drinking water has been provided, there are micro-organisms that are resistant to inactivation or disinfection process that survive and multiply within water distribution systems

(Sekar et al. 2012). Microorganism's occurrence in water distribution system (WDS) combined with favourable growth conditions for bacteria may lead to bacterial regrowth. Bacterial regrowth has been associated with coliform occurrence, the likelihood of waterborne illness, enhanced pipe corrosion, and taste and odour problems (Zhang et al. 2004). Each WDS is a complex system that consists of hundreds or thousands of individual pipe sections where numerous factors (e.g. characteristics of substrate, water temperature, concentration of residual disinfectant, etc.) impacts the bacterial regrowth, therefore it is very difficult to explain the bacterial regrowth, for example, by a heuristic approach such as multiple regression analysis of observations made at monthly intervals at various stations throughout a WDS (Zhang et al.2002). Based on complexity of the predictions of bacterial regrowth in WDS there has been a mathematical models developed to make the predictions accurate.

The aim of this paper is to analyze the history of the water quality modelling and understand the challenges of water quality modelling in future.

THE FIRST GENERATION MODELS

The first generation models has begun to appear in literature in middle of 1990`s (Servais et al. 1994; Camper 1996; Dukan et al.1996; Bois et al. 1997). All of these models described in literature are based on mechanistic models of biofilms in water and wastewater treatment processes. Overall review of these models is summarized (Gagnon et al. 1997), the main conclusions is that these models where too complex to expand them to whole WDS.

Servais et al. (1994) and Bois et al. (1997) have developed two independent but very similar models. Those models can describe the growth of the attached bacteria (biofilm), the growth of free or suspended bacteria in bulk water, the loss of substrate, the inhibition of growth by chlorine and the loss of chlorine by oxidation reactions. Although the description of biological and chemical processes was decent, there were a large number of constants that had to be specified to run the model. The other drawback of the models was that the chemical and biological processes are not linked with a hydraulic model. Since the hydraulics of the WDS has a great impact on bacterial regrowth (Rice et al. 1991; Brazos et al. 1982; LeChavallier et al.1987) this has been considered as a serious drawback.

Camper et al. (1996) has developed the biofilm accumulation model (BAM), the aim of development of this model was to provide detailed description of biological and chemical processes in pipe lines. The model consisted of only one pipe; it means that it was not suitable for modelling of bacterial regrowth in whole WDS. It also was not linked to any hydraulic parameters.

Model developed by Dukan et al. (1996) (PICCOBIO) in comparison to previous models contains the possibility of coupling of steady-state hydraulic conditions with the biological and chemical reactions. However, it was still too short to provide a dynamic bacterial regrowth results for at typical unsteady-steady condition WDS.

THE SECOND GENERATION MODELS

The second generation models have been developed in beginning of 20th century (Rossman 2000; Zhang et al. 2004, Shang et al. 2007; Shang et al. 2008). In development of second generation models the bacterial and chemical reactions are coupled with the hydraulics of the WDS.

Rossman (2000) have developed the EPANET model. Although, it is not the bacterial regrowth model, it is a widely used, public-domain model that performs extended period simulation of hydraulic behaviour within pressurizes pipe networks and also includes a single chemical species

(Rossman 2000). This model captures the dynamics of the transports and transformation of a chemical species under unsteady-state flow conditions as would be typically encountered. The most common water quality application of EPANET is to predict chlorine concentration given that it undergoes first-order decay in the bulk water and either first- or zero-order decay (under specified) at the pipe wall (Zhang et al. 2004). If the biological and chemical processes are coupled with the hydraulic processes in the WDS, the mass transport simulation schemes should be used. The EPANET uses the Lagrangian time-based approach to track the fate of discrete parcels of water as they move along pipes and mix together at junctions between fixed-length time steps (Rossman 2000). This kind of approach considers that there is only advective mass transport in pipes; it means that bulk species are transported down the length of a pipe with the same average velocity as the carrier fluid while at the same time reacting with the other bulk species (Shang et al.2007). This is a drawback of the EPANET model because it does not include hydraulic dispersion or diffusion as a transport mechanism. This may be not a problem when there are high water velocities in pipes, but when there is low flow conditions in WDS and low water velocity in pipes, the mass transport into the pipes could be dominated by dispersion of diffusion (Axworthy et al. 1996). Other drawback of the model is the assumption that there are complete and instantaneous mixing in pipe junctions and reservoirs (Shang et al. 2008).

On the basis of EPANET there is developed an additional software EPANET-MSX (Multi-Species Extension) for solving drinking water quality variations in WDS. This software uses the hydraulic parameters from the network built in EPANET and couples with the biological and chemical reactions set up in EPANET-MSX. Extension allows implementing ordinary differential equations (ODEs) for solving the reactions. The EPANET-MSX system provides an investigative tool that allows engineers, chemists and microbiologists to collaborate to advance the state of knowledge of water quality in WDS (Shang et al.2008). Since the hydraulics of the model is linked to EPANET it still has the same drawbacks as EPANET.

Zhang et al. (2004) has developed the model for predicting the bacterial regrowth and transport for attached and free bacteria, biodegradable dissolved organic carbon (substrate) consumption and transport, chlorine decay in bulk water. In comparison to EPANET model, the advective-dispersive transport mechanism is used in proposed model. A major advantage of the method that have proposed by Zhang et al. (2004) is that it can provide good descriptions of concentration profiles in distribution systems for any extent of dispersion, unlike traditional low-order finite difference methods and Lagrangian methods that ignore dispersion. This model has not been tested under dynamic hydraulic conditions as would occur due to diurnal variations in water demand in WDS, there should be some additional investigations done (Zhang et al.2004). Some attempts to implement the model for real scale WDS has been done, for example Rubulis et al. (2007) tried to use the model for simulating the bacterial regrowth in Riga city WDS. The results showed that constants used in model should be reviewed as well there should be some coefficients added for phosphorous utilization modelling (Rubulis et al. 2007).

The second generation models is a huge step forward to an accurate prediction of the bacterial regrowth and chemical reactions in WDS, however, there are issues related to solving the mass transport for biological or chemical material in WDS.

IMPROVEMENTS FOR MASS TRANSPORT IN WDS

To solve the water quality modelling drawbacks there are several studies done, the main objective of the studies is to improve the equations and solvers that provide the modelling of mass transport in WDS. The studies can be divided in two sections: the studies related to axial mixing, advection, diffusion, dispersion in straight pipes and mixing in junctions.

Axial mixing models

The dispersion-diffusion process in drinking water quality modelling plays more important role if transport of conservative contaminants is modelled. If the reaction rates of the contaminant increases, the dispersion-diffusion process becomes relatively less important (Tzatchkov et al.2009). However, in low flow conditions the role of the dispersion-diffusion should be taken into account.

The advection-reaction models fail to properly represent the observed concentration in the pipes where low velocities prevail; low velocities are caused by varying flow conditions during the day, the minimum pipe diameter requirement, dead ends, and other factors (Tzatchkov et al. 2002, Buchberger et al 2003). For example, a study of a WDS in Mexico, using hydraulic simulations and field measurements, indicated that low flow velocity is presented in 66% of the network pipes (Hansen-Rodriguez 1997). Another study has shown that about 23-35% of the total WDS can be considered as dead-end pipes and that depending on the time of the day, low flow conditions may predominate in 20-50% of a WDS (Buchberger et al 2003). Based on tracer tests performed in the WDS of Riga city Latvia (1374 km, 700 000 inhabitants, average daily water demand of 1500 l/s) the average modeled velocities in peak hours ranged from 0.13-0.30 m/s (Rubulis et al. 2010). Since this tendency is very significant, the dispersion and diffusion processes must be taken into account for water quality simulations (Tzatchkov et al. 2002).

To improve the mass transport simulations in WDS Tzatchkov et al. (2002) proposed a new two steps solving transformation scheme based on Eulerian-Langragian method and classical Taylor (1953, 1954) theory of dispersion. Through the first step, a transformation of the dependent variable makes the advetion-dispersion-reaction (ADR) equation become one equation where only advective and dispersive terms are present. Through the second step, a transformation of a spatial coordinate to one that follows the characteristic curves of the advective operator gives the differential equation a purely dispersive character. As investigational subjects of water quality, fluoride and chlorine concentrations were selected. The resulting simulations compared to the simulations run with the EPANET model and observation showed that in network pipes with the medium and high flow velocities the results are similar. However, in the pipes with low flow velocities ($v < 0.02$ m/s), the observed concentrations are more closely to proposed model. Although, the results were more precise, it required much more computing resource and some more studies should be done to improve the solver that it could be applied for real scale WDS (Velitchko et al. 2002).

Romero-Gomez et al. (2011) proposed to improve the classical Taylor Taylor (1953, 1954) theory by implementing two dispersion coefficients, one for the dispersion in the front of the tracer (contaminant), and other for the dispersion in the downstream of the tracer. This assumption was based on the experiments done in pilot scale WDS, where the presence of solute tailing long after a tracer pulse has passed a fixed downstream location revealed that the dispersive rate toward the end of the pulse is stronger that the rate near the front. The measurements where done for electrical conductivity, and in laminar flow conditions ($v < 0.13$ m/s, $Re < 2000$). The 1 dimensional ADR model was made. Obtained modelling results were very close to the experimental results. The drawback of this model is that it has been made for single pipe simulation, it has to be combined with the efficient numerical schemes that are used to analyze real scale WDS.

Solute dispersion is an important component of WDS water quality simulation, and it should be incorporated into the next generation of WDS quality models (Tzatchkov et al.2009). Those models should be integrated in 1-D-Advection-Dispersion-Reaction model mechanisms that are widely used for real-world WDS system analysis (Andrade et al. 2011). This kind of improvements would lead to more accurate water quality predictions, what may lead to more precise risk assessments, especially for system regions with low-velocity flows.

Mixing in junctions

A numerous studies during the last years has shown that there is no perfect mixing at pipe junctions and studies clearly have demonstrated that the perfect mixing assumption in water quality models can produce considerable errors in water quality modelling (Machell et al. 2007, Romero-Gomez et al. 2008, Austin et al. 2008, Choi et al. 2009). There have been several attempts to improve the models to achieve more precise modelling results.

Choi et al. (2009) has developed a comprehensive solute mixing model AZRED, which is suitable for modelling mixing at double-tee, cross and wye junctions in WDS. To develop the model there were a series of experiments conducted. Obtained experimental results afterwards are applied in the model code. The model code is based on the EPANET model. The modified code takes the original incoming pipe concentration values and applies the experimental data in order to calculate the modified outgoing pipe concentration values. Then it replaces the original perfect mixing (assumed in EPANET model) with the modified non-perfect mixing values. These improvements are capable of handling incomplete mixing at various types of 4-way junctions such as crosses, double-tees and wye connectors (Andrade et al. 2011) Achieved modelling results were much closer to the EPANET model results. However, there are some limitations for AZRED model, the ratios of the Reynolds number are based on experimental results, and the ratios approaching zero or infinity are extrapolated from experimental data; consequently, approximation may not be completely accurate. Also, unequal inlet and outlet pipe diameters at junction may introduce errors (Choi et al 2009).

It is widely known that water age, as defined by the cumulative residence time in the system, is considered a reliable surrogate for potable water quality (Choi et al 2009). Based on that, Machell et al. (2007) has developed the water quality model based on water age calculation. An improved model tracks water age within user defined bounds for WDS. It is proposed that water age is calculated and monitored throughout networks through assignation within defined age bands. The bands can be set by the user. The method determines the percentage of the flow from each pipe merging at a node that falls into each of used defined bands, and that fall outside the chosen range assuming complete mixing within a given band (Machell et al 2007). The shortcoming of the method is that it is only suitable for calculation of water age into the system and it is not applicable for modelling of contaminant spreading in WDS; however, improved code of the proposed method could be applied for wide range of contamination mixing simulations in WDS. The advantage of the method is that requires significantly less computational resources than other proposed methods.

Although, there has been developed several new methods for modelling water quality mixing at junctions, none of them is right away usable for high precision water quality simulations. The models should be improved and included in most common water quality modelling tools, as one of the solutions to calculate large range of data can be usage of high performance computers.

CONCLUSIONS

During last year's there has been a significant progress in water quality modelling in WDS. Although a numerous studies done, there has not been any user friendly high precision tool made. All of the studies showed that the models that have been widely used for last 15 years should be improved more.

The mass transport solving methods and equations regards to advection-dispersion-reaction must be improved to achieve more precise results for water quality modelling in pipe sections. Also water mixing description in junctions is not precise enough. The studies that have been done in most cases lead to complicated models that require a lot of computing resources if the real scale system should be analyzed. After improvement of those shortages, the water quality modelling would be a useful tool for utility managers and water resource engineers who work in next generation network design of water distribution systems, operation, real-time sensor optimization and placement, contingency planning and network security, and risk assessment.

All of the studies done about mass transport development, has been done with chemical substances, it means that there are wide field of studies to be done with biological matter transport in WDS. Since the methods for bacterial mass or amount analysis needs several days, the validation and verification of such a models will take a very long period of time. Also the reactions and biological regrowth is very complicated and individual processes for different kind of biological matter, that should be simplified and generalized enough to meet the requirements of precision of the model and the time and computing resources that is needed. To minimize the time consumption for experiments and modelling is the greatest challenge for the drinking water quality modelling of biological regrowth.

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