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Models for drinking water treatment processes

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Abstract. With drinking water standards becoming more rigorous and increasing demands for additional water quantities, while water resources are becoming more polluted, mathematical models became an important tool to improve water treatment processes performance in the water supply system. Water treatment processes models reflect the knowledge of the processes and they are useful tools for water treatment process optimization, design, operator training for decision making and fundamental research. Unfortunately, in the current practice of drinking-water production and distribution, water treatment processes modeling is not successfully applied. This article presents a review of some existing water treatment processes simulators and the experience of their application and indicating the main weak points of each process. Also, new approaches in the modeling of water treatment are presented and recommendations are given for the work in the future.

Keywords: active control; dynamics; granular materials; water quality; water treatment; plant; process modeling

1. Introduction

Water utilities are required to provide additional quantities of drinking water, which must comply with increasingly stringent standards for drinking water quality, while at the same time the sources for the water supply system are becoming increasingly polluted.

As the quality gap between the raw water and drinking water is increasing, more energy and/or chemicals are required to achieve the water quality with respect to the drinking-water standards (Bakker *et al.* 2014). At the same time, more energy and chemicals lead to a more negative impact on the environment (more sludge and wastewater, etc.). It has been estimated that 15% to 20% of the supplying potable water cost is incurred at the treatment stage (Van Schagen 2009). The costs can be significantly decreased and the environment will be protected if water treatment is optimized. These optimizations will strive to achieve acceptable water quality on a continuous basis while minimizing capital and operational costs, and the negative impact on the environment.

In order to stay competitive in the market, water utilities are looking for solutions to be able to

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make predictions on how their treatment processes can be improved (Jusic and Milasinovic 2015). To increase the efficiency and provided a better and more stable water quality, water supply companies are gradually moving towards a centralized and fully automated operation (Angreni 2009). Fully automated treatment plants will require a more sophisticated staff – operators than manually operated plants, so operation supervisors should conduct periodical trainings for the usage of these programs/models for control of the utility performance. Models are an essential part of the simulators since they denote the behavior of the treatment plant's processes.

Models can be categorized in different ways, including (Jakeman *et al.* 2017):

- type (e.g. empirical, conceptual, physical, numerical, analytical models);
- treatment of space (e.g. non-spatial models, lumped spatial models, grid spatial models);
- treatment of time (e.g. non-temporal, steady state, lumped discrete, dynamic);
- composition (e.g. coupled/unit, integrated);
- execution (e.g. distributed, web-based).

Various factors influence the modeler's choice regarding the most appropriate model.

Unfortunately, the application of models in the daily operation of the treatment plant is not a simple task.

2. Conventional water treatment processes and modeling

2.1 Conventional water treatment processes

Although some water sources could achieve the required improvement in water quality through the application of a single treatment process (disinfection mainly), it is more common to apply several complementary processes (Akinmolayan 2017). As a "treatment train", conventional drinking-water treatment plant consists of many processes/units: coagulation-flocculation, sedimentation, filtration through granular materials and disinfection. Fig. 1 illustrates the flowsheet of conventional water treatment processes. In a conventional water treatment plant, the main processing units are connected by pipes or troughs.

As mentioned earlier, regarding composition, two levels of process simulation (modeling) exist, the unit and the integrated one. By connecting different unit models a complete drinking water treatment plant can be simulated by integrated modeling. The former is designed to simulate the whole water treatment in the operation mode, while the later provides support in the optimization process and design of single process/unit steps. So, for different processing units, individual/unit models exist. In order to combine/integrate these individual models into a model for a complete treatment plant, connections between each unit have to be made. The outlet concentration from the individual processing unit models is equated to the inlet concentration of the next unit model of the integrated (pipeline) model, as illustrated in Figure 2. Flow rate will flow along the length of the pipeline, then the effluent concentration from the pipeline ($C_{p,in}$) is equated to the inlet concentration ($C_{p,\, out}$) and flow for the following unit. The outlet concentration ($C_{A,out}$) from the individual processing unit model is equated to the inlet concentration ($C_{B,\, in}$) of the "pipeline" (integrated) model (Fig. 2).

The parameters of the process can be grouped into input (design), operational/manipulative and output/control parameters (concentrations) (Imamovic *et al.* 2015). Typically, the output consists of water quality parameters that are relevant for the process and other data that describe the state of the process. Calibration parameters should be defined in the modeling process as well. All these

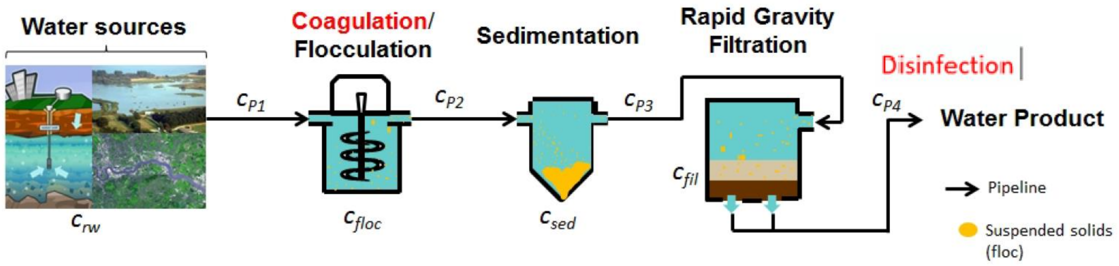

Fig. 1 Illustrative flowsheet of conventional water treatment processes (the physical processes are labeled in black color and the chemical processes in red color) (Akinmolayan 2017)

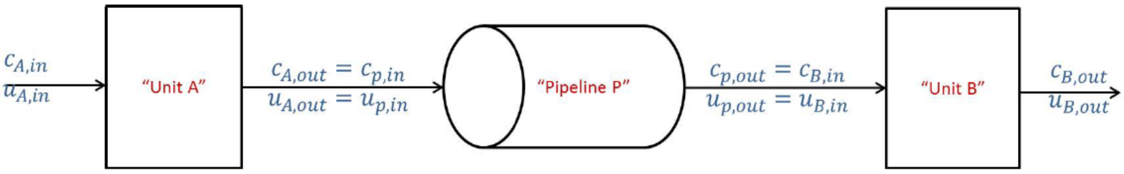

Fig. 2 Illustration of the individual mathematical model connection with the pipeline (integrated) model (Akinmolayan 2017)

Table 1 Rapid sand filters – Overview of relevant parameters for Stimela modeling (Jusic and Milasinovic 2015)

Parameters of Filtration		
Input –	Design:	filter surface area, filtration rate, filter bed height, number of bed layers, water level above the filter bed, filter porosity, grain size
	Disturbance:	water flow, the concentration of pollution (suspended solids, turbidity), temperature
Operational or manipulative:		*filtration cycle time/filter run time*, backwashing time, start time for backwashing of filter granular materials
Output – Control:		the concentration of filtered water pollution (suspended solids i.e. turbidity), disposition of pressures in the fill (pressure losses)
Calibration:		Lambda*– coefficient of filtration, clogging constant, the mass density of the flocks, number of completely mixed reactors

* Lambda is a term that is used in the *STIMELA* environment, and it represents the coefficient of filtration of the collimated fill. It is one of the calibration parameters which is in function of porosity, water velocity and transfer coefficient (Rietveld 2005)

parameters are determined by the characteristics of a particular plant or operation. For example, relevant parameters for the process of rapid sand filtration are presented in Table 1.

Appropriate changes in operational and input design parameters allow more efficient use of the existing capacity of the processes and better active control of risks and uncertainties. The aim is, by varying values of operational or input design parameters to understand how these parameters influence the output. Additionally, simulating the impact of such changes, for example, the operational parameters on the output can support the operator in the decision-making process for better plant operations management. The model needs to have the ability to estimate the parameters of interest for the process/unit at the right scale and resolution (i.e., temporal, spatial, and thematic) which matches the rate of change in the system of interest (Ibrahimbegovic *et al.* 2016). The phases of modeling can be described as:

- scoping (model study plan including identifying model parameters, purpose and study objectives);
- problem framing and formulation (including conceptualization);
- analysis and assessment of options (model setup, and calibration and validation) and
- discussion of the results (of simulation and evaluation).

2.2 Modeling of water quality in water treatment - purpose and objectives

Within a perspective of sustainable development, treatment plants must be designed on the basis of technical, economic and environmental criteria (Yoann 2013) (Jakeman *et al.* 2017). Information Technology (IT) tools for water treatment modeling will form the link between data, model, active control, research, education/training and design (Figure 3). The knowledge of operators, designers and researchers is based on different information. Operators get information from the full-scale plant, while designers obtain their data from pilot plants and researchers from experiments on the lab-scale (Rietveld *et al.* 2004). Calibration or testing of models is performed experimentally by measuring the corresponding data on the pilot plant or the actual plant. Frequently pilot plants are available for calibration and validation of the models, while in full-scale plants the models can be tested and used for the improvement of the processes.

Obtaining a model is never a goal in itself (Ani 2016). There is always a purpose for obtaining a model. Models for water treatment processes can be used for different purposes:

- understanding of processes;
- optimization of design;
- optimization of process control (active control);
- predictions of the treatment plant performance under changing conditions (scenario studies).

Models for water treatment processes include simulation, i.e., modeling of water quality, flow hydraulics, process controls and design (determination of design process parameters). The quality of drinking water is an important matter, because water of low quality may cause health-related and economic problems which have a considerable impact on people’s daily lives (Jakeman *et al.* 2017). *The water quality model* is a mathematical representation of the pollutants’ transport. This

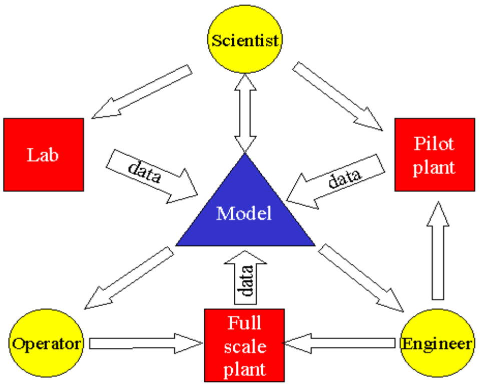

Fig. 3 Linking research to design and training (Rietveld 2004)

model tries to simulate changes in the concentration of pollutants as they move through the water treatment plant. The *hydraulic modeling* software package (EPANET) is used worldwide to design water distribution networks and to optimize their operation, up to complete integration with the SCADA systems (Ulinici *et al.* 2014). However, in the current EPANET library, the elements that describe the hydraulic properties of some water treatment units are missing. These elements have to be more developed and integrated, which has to be based on modeling of unit processes performed in the first stage.

In many cases, the purpose of modeling is to optimize the control of the processing analysis and to optimize the design parameters. Models used at this stage are models for simulation of control and design parameters of the process. In the process analysis, one wants to predict the process behavior in certain circumstances. By modeling, it is possible to conduct a rapid and inexpensive analysis of a large number of alternatives by changing the operational/control or design input data of the water treatment process following the impact on output/control parameters. In this way, modeling enables one to select appropriate design or control parameters (Rietveld 2005).

By modeling, it is possible to obtain a better understanding of the process, by increasing the insight how different parameters affect the efficiency of the process. The purpose and objectives of a model should include a clearly articulated set of user data requirements, processes that should be represented, questions, functionalities, system boundaries and predictive quantities of interest.

A few existing modeling environments of water quality in the water treatment are briefly explained in the next chapter.

3. Water treatment processes modeling environments – a review

Many commercial software programs are able to model the performance of water treatment processes/units that have been produced. Existing software packages for modeling and simulation of processes offer, more or less, the same functionalities: design, process optimization, operator training, process fundamental research (Jusic 2015). These conventional programs are generally similar in terms of their application, allowing different processes to be combined (integrated composition) (Fig. 4). Each of the water treatment modeling packages has its specific characteristics (Dudley *et al.* 2008).

OTTER contains models for most commonly encountered processes and less conventional processes may require the development of a suitable mathematical model. *OTTER* has been used throughout the world, but predominantly in the UK and the USA. Typical usages of the software include operational decision support, works optimization, plant design, and operator training. Several studies have been carried out using *OTTER* at waterworks (Butler 1998, Gallis 1999, Giraudet 2002a, b, Guo and Sankararamkrishnan 2003, Jusic 2016). Generally, all of these have been successful, however, they have highlighted the requirement for relatively large data for successful calibration and use. The empirical nature of the coagulation and flocculation models indicated that the calibrated models could not be applied significantly outside the calibration region, restricting the degree of optimization that could be studied.

The main purpose of *Stimela* is to support research and development, and active control applications. Therefore, it focuses on model development, it is an open-source programming platform, and the graphical output is flexible. *Stimela* is an environment where different drinking-water treatment processes can be modeled dynamically. The models of individual/unit processes

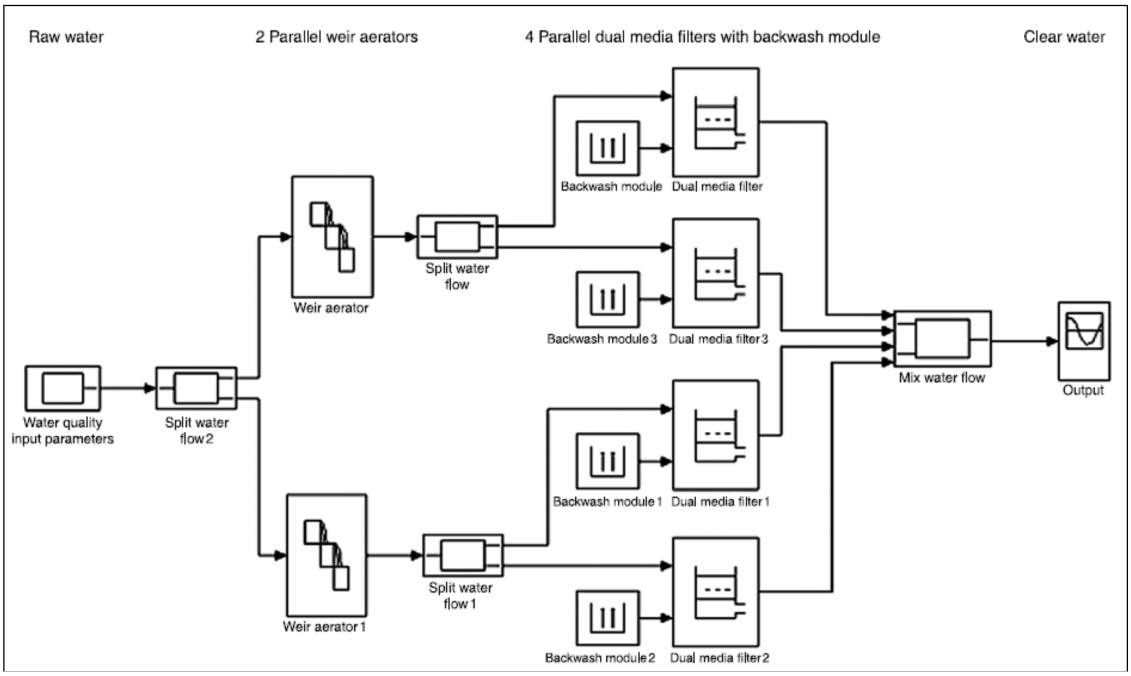

Fig. 4 Example of connection of the unit model into an integrated model – *Stimela* environment (Dudley *et al.* 2008)

are situated in a model library and can be connected to each other, forming an integrated model "treatment train" (Fig. 4). In this way, the effect of operational changes in preceding treatment processes can be evaluated (Campos *et al.* 2006). The flowsheet model can be run after specifying all the parameters, choosing the integration method, the step size and the simulation time. After the simulation, graphical output is obtained by opening the output block. The calculated values can be compared with the measured data.

Metrex was developed mainly to examine the use of particle size distribution as a modeling approach to better understand the particle removal processes, rather than general water treatment. It requires the collection of a higher amount of data. *Metrex* was developed at the University of Duisburg, Germany (Rietveld *et al.* 2009) and it is not being actively developed now. It combines analytical and numerical models of common treatment steps used in the surface water treatment. The emphasis is on the particle removal (particle size distributions are considered) and ozonation (oxidation of dissolved organic carbon, iron and manganese, and formation of bromate).

The *WTP model* was originally developed by the United States Environmental Protection Agency (US EPA). The *WTP model* was developed to model disinfection and disinfection of by-products in support of the Disinfectant/Disinfection By-products Rule. It models the general case rather than site-specific conditions and is not designed to replace site-specific studies. It is mainly used for the evaluation of design rather than for optimization and is utilized by experienced engineers. The *WTP model* is based on empirical relations obtained from the regression analysis. It was prepared with the understanding that the predictions should reflect typical average performance values, and is focused on the removal of natural organic matter (NOM), the formation of Disinfection by Products (DBPs) and disinfection.

Table 2 Summary characteristics of available programs (Rietveld *et al.* 2009) (Ulinici *et al.* 2014)

CHARACTERISTICS:	*OTTER*	*Stimela*	*Metrex*	*WTP*	*WatPro*
Dynamic?	Yes	Yes	Yes	No	No
Sludge processes?	Yes	No	No	No	No
Recycles?	Yes	Yes	No	No	No
Disinfection models?	Yes	Yes	Yes	Yes	Yes
Clarification?	Yes	No	Yes	No	No
Filtration?	Yes	Yes	Yes	No	No
Easily extendible?	No	Yes	No	No	No
Engineering use?	Yes	Yes	No	Yes	Yes
Research use?	No	Yes	Yes	No	No
Easy to use?	Yes	No	No	Yes	Yes

WatPro is supplied by Hydromantis Inc. (Rietveld *et al.* 2009). *WatPro* is effective at modeling the chlorination by-product formation. It is a steady-state water treatment modeling program, with a focus on disinfection and disinfection by-products. Although other aspects of water treatment processes are supported, these are of lesser significance within the package's scope.

TAPWAT (Tool for the Analysis of the Production of drinking WATer) is developed by the Netherlands Institute of Public Health and the Environment (RIVM), with the following goals:

- To predict on a global scale, the quality of drinking water (including health risks levels by micro-organisms) given a certain raw water quality.
- To advise the drinking-water inspectorate by reviewing new or renewed production plants especially concerning public health risks (Rietveld 2005).

The main purpose of *TAPWAT* is to determine the probability of occurrence of pathogenic micro-organisms and DBPs in the product of a treatment plant, consisting of different steps in the series.

Table 2 presents a review of the basic characteristics of the above-mentioned models for water treatment. The ability to models certain characteristics is answered by positive or negative answers.

4. Water treatment model application

The existing modeling environment was found to have varying availability and documentation. Processes modeled were also skewed towards those prevalent in the country where each program was developed (Juntunen *et al.* 2012). Unfortunately, there has been little use of water treatment models, especially in comparison with wastewater programs. Drinking-water modeling (developed in the 1990s) is thought to be less developed and applied than wastewater modeling (developed in the 1970s) due to the amount of time they have existed (Ulinici *et al.* 2014). Also, mathematical analysis of the drinking-water modeling is not a mature scientific discipline as possibly expected. As a general tool that can be of assistance in improving water treatment, the modeling of water processes has confronted many challenges (Serdarevic and Dzubur 2016). Since the drinking-water treatment processes involved are physically and chemically heterogeneous, the water and process parameters are generally complex and their mutual interactions nonlinear. The drivers for

Table 3 Summary of recent filtration models and their strengths and weaknesses (Akinmolayan 2017)

Models	Strengths	Weaknesses
Detachment mechanisms	It can simulate filter performance satisfactorily and easily for all filtration velocities.	The inclusion of factors relating to the attraction in the transient state modeling in an explicit manner is required.
Filtration and adsorption	It can simulate filter performance satisfactorily.	Only for low filtration velocity.
Retained particles blocking another particle collection	Based on the random sequential adsorption mechanism, which can be used to predict the transient stage and deposition of colloids.	Cannot be applied for unfavorable surface condition.
Effects of the change in the surface change of filter grains	Useful in predicting the accumulation on the filter grain surface due to the deposition of particles.	The model is valid in predicting the changes in the filter granular materials structure only at low inception numbers.

the transport of the solutes and particulates (pollutants) are the velocity of the flow (advection) and dispersion for water quality models. Whereas the drivers for the hydraulic model of water flow are potential energy or pressure head differences. This means that calibrating a model for water flow does not necessarily mean that this will work well for solutes and particulates (pollutants). Furthermore, successful applications of traditional models are limited to idealized, artificial systems, so the correlation between the simulated and experimental data from the real processes has been poor and expensive *in situ* testing is needed.

For instance, there is an agreement on the fact that coagulation modeling is still an issue for water engineers (Rietveld *et al.* 2009). This unit process is designed with the application of rules of thumb and basic experimentation (e.g. jar-test). The corresponding models are data-driven and spite-specific. Models for DBPs formation contain empirical equations requiring extensive data for calibration. Regarding the filtration process, as a process in porous granular materials, there is a variety of unit models that have been developed to calculate the particle capture in a filter (Kowalsky *et al.* 2014). Although filtration models can be used very effectively to assess the influence of each parameter, such as filter velocity on filter performance, they all have several weaknesses (Tasiopoulou *et al.* 2015). Table 3 presents a summary of the most cited models found in the literature which predict the removal efficiency during the transient condition of a filter and lists their strengths and weaknesses.

The balance between empirical approach and formal mathematical modeling must be reconsidered in the water treatment simulation. There is a need for more mechanistic (dynamic and integrated) models. Also, one of the main problems regarding the existing work on dynamic modeling water treatment processes individually is a lack of understanding as to how these unit models fit together to develop a complete water treatment plant (integrated). Knowledge and understanding of individual processes (unit models) can facilitate their connection and formation of an integrated model of all water treatment plants.

The water treatment modeling was rarely used, due to the need of an extensive quantity of data required for calibration of the (empirical) models (especially coagulation models) and the fragility of the models when applied outside the calibration region (Ottenheijm 2016). Additional limitations for the implementation of these models exist.

- Firstly, ideal conditions are often assumed which will have an effect on the predicted concentration once the units have been combined to make an integrated water treatment model. The individual unit model will behave in an ideal way. Expansion by the integration of the individual models (integrated models) will result in some limitations.
- Secondly, due to the nature of the unit process models, empirical parameters are needed for accurate simulation of a process on a specific site, which requires experiments or historical data to find empirical relationships.
- Thirdly, ss the current work on dynamic modeling of water treatment processes is considered as separate units, it is, therefore, therefore lacking a complete understanding of how these models behave/fit together in an integrated water treatment model.

All simulations are subject to uncertainty having in mind that the hydraulics, input (disturbance and transport) parameters and boundary conditions are never known insufficient details. In the previous section, an overview of the existing modeling environment was provided. Although useful as a catalog it does not provide any independent guide regarding the quality of the models. The "best" model does not exist: selection is a function of the application and questions to be answered (Pinto *et al.* 2009).

With the aim to improve the application of water treatment process modeling in recent times there are new trends, which are briefly explained in the next chapter.

5. State-of-the-art in water treatment modeling

The goal is to develop meaningful, credible models from available data and prior knowledge that will be beneficial for the end-users (operator, engineer or scientist). These models will be open to critical review and revision in every stage. Unfortunately, mathematical modeling is perceived as an academic exercise as opposed to field operations (it is remote from the issues faced by water engineers working on the field). Recommendations that require specific attention in the water modeling domain, with the aim of its better application, are the following (Jakeman *et al*. 2017):

- Emphasize effective simplification over undiscerning and unnecessary model complexity, especially where complexity reduces transparency, increases uncertainty and/or hinders its assessment.
- Educate users about model results about the dangers of being provided only a single number upon which to base their decisions - but also address their needs, by providing uncertainty information in a format that fits within their workflows.
- Communicating uncertainty is an area of emerging attention that could be advanced by focusing on meeting its challenges in the water sector. Visualization of indicators that are of importance is an aspect of such an endeavor.
- Pay explicit attention to the way the model's results and uncertainty are communicated in written reports and publications.
- Make effective use of user-centered design for visualization development early in the modeling process, and leverage different visualization tools to engage different audiences (e.g., researches, policymakers, stakeholders).
- Embrace the use of automated methodologies that can support both the transparent experimental workflows and allow for systematic understanding of the impacts of the various relationships and factors that influence the model's results.
- Pay careful attention to the collected data, including measuring the right variables, at the right

locations, and with the right frequency.

The issue explained in the previous chapter, must be tackled while developing the next-generation IT (Information Technology) tools for water treatment modeling (Rietveld 2005). The first stage of this software development, a state-of-the-art review of the existing water treatment simulators, has been carried out to identify what would be needed for a new system - integral modeling of drinking-water treatment (Akinmolayan 2017). Numerous new trends of other tools for water treatment simulation exist (Swan *et al.* 2016). Some of them are *EVALEAU* research project, *TECHNEAU*, Artificial Neural Networks (ANNs), "surrogate" models, ect., which are briefly explained in this chapter.

The global objective of the *EVALEAU research* project was to develop an IT tool for multi-criteria decision support in the field of drinking-water production (Yoann 2013). Three main steps of this project were the development of a model library for unit processes; integration in a computer framework enabling plant flowsheet and development of a toolbox for mathematical analysis in order to support the eco-design activity. The development of the *EVALEAU* tool necessarily relies on a multidisciplinary approach, combining very different domains: process engineering and water treatment, environmental assessment, applied mathematics, and software engineering.

The EU-funded project, *TECHNEAU (Technology Enabled Universal Access to Safe Water*), intended (among other tasks) to develop a new water treatment simulator (Hoven and Kazner 2009). Before starting with any software development, a review of the existing water treatment simulators was done, to identify what is required for a new system. The simulator will incorporate aspects of the existing software as well as the implementation of the new process models to be developed within *TECHNEAU*. *OTTER* and *Stimela* were selected as the basis of the framework for the new water treatment simulator to be developed as part of *TECHNEAU*. This very flexible modeling environment enables the user to integrate additional knowledge in the model library and to use it as a collaborative platform for research and development.

For a model of water treatment plant (processes integrated) to be fully utilized, it is required to be operator friendly, and the detailed mathematical models shown so far are rather complex and the simulations require professional software and computational capabilities. With this in mind, the new trend addresses the development of simpler, or "*surrogate*" *models*, which are easier to use and require less sophisticated solution methods (Razavi *et al.* 2012). "Surrogate" models, developed through the regression analysis, are black-box models that are generated from data either sourced experimentally or obtained from a highly-accurate and computationally expensive models. Simplified "surrogate" models are generated by detailed models but with less complexity which will, therefore, reduce the computational expertise and time needed.

The use of artificial networks (ANN) in plant control or for resource planning in water treatment is very limited. Models will always carry a certain amount of risk and error but this is no different from lab sampling. It is, however, the limitation of the ANN models in the plant control systems lies in the inability to verify the error that is made by the ANN. There are endless possibilities for the use of ANNs in water treatment. The performance and accuracy are, however, very much dependent on the quality of the dataset and the chosen model structure. A key risk in ANN development is overfitting or underfitting the data.

Predictive modeling is a process used in predictive analytics to create a statistical model of future behavior. Predictive analytics is the area of data mining concerned with forecasting probabilities and trends (Pinto 2009). On the other hand, Artificial Intelligence (AI) concerns itself with intelligent behavior, i.e., the things that make us seem intelligent. Following this process of thinking, the main goal is the assessment of the impact of using AI based tools for the development of intelligent predictive models, in particular, those that may be used to establish the conditions in which the levels of manganese and turbidity in water supply are high.

By *PROMICIT project*, which started in 2003, Amsterdam Water Supply (AWS) implemented the change in the research philosophy. AWS in cooperation with the Delft University of Technology already developed several process models for individual processes. These models are integrated into the *Stimela* environment, which is programmed in Matlab/Simulink (Rietveld et al, 2009). These models will be extended and will be integrated into an overall process model - Integral modeling of drinking-water treatment. Through this project, in the future, the drinking-water treatment will be automated. Data will be collected online and sent to the *Intelligent System (IS) of the treatment*. The IS will propose a treatment strategy based on the defined goal factors e.g. the required quality and cost. Models are the basis for the IS and will be an interface between the data and the active control of the water supply. These models are a reflection of the knowledge of the system and are fed by data and (new) hypotheses. This will lead to cost-effective, high performance, stable and reliable treatments.

6. Conclusions

Using models for evaluation of the treatment processes can increase the knowledge and enhance the exchange of knowledge. This will be a step forward in the optimization of plant performance and thus improvement of drinking-water quality. The modeling of water treatment processes is challenging due to its complexity, nonlinearity, and numerous contributory variables, but it is of particular importance since the water of low-quality causes health-related and economic problems which have a considerable impact on people’s daily lives.

Although continuous progress in recent years is being made in improving the accuracy of mathematical models to predict water treatment processes, additional research still needs to be carried out. To ensure the successful implementations of mathematical models in the water industry, regulators, water companies and modeling experts need to come together to develop formal guidance on good modeling practices that describe how models must be used in water companies.

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