WATER TREATMENT SIMULATORS: STATE-OF-THE-ART REVIEW

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ABSTRACT

A new water treatment simulator will be developed as part of the EU-funded Integrated Project TECHNEAU (Commission of the European Communities, Research Directorate-General: Technology Enabled Universal Access to Safe Water, Contract No. 018320). The simulator will incorporate aspects of existing software as well as the implementation of new process models to be developed within TECHNEAU.

The first-stage of this software development, a state-of-the-art review of existing water treatment simulators, has been carried out to identify what would be needed for the new system. This review has identified that there has been little usage of water treatment modelling, with the two main objections being the quantity of data required to calibrate the models and the fragility of the models when applied outside the calibration region.

INTRODUCTION

Although drinking water treatment has a long history, the mathematical analysis of these treatment processes is still young. Many flocculation ‘models’ are data-driven (e.g. Baxter *et al.*, 2002) and are difficult to generalise to other treatment works. Other treatment processes, such as disinfection and filtration, have been widely studied and the models are on a sounder basis.

To enhance the ease of use of these models, they have been linked together in flowsheeting programs. Flowsheeting programs started in the chemical industry in the 1960s, and in wastewater in the 1970s, but it was not until the 1990s that they were really applied to the water industry. Part of the reason for this has been the slow growth in the number of available models, so that there was no need to have a program that would allow the different models to be readily chained together. Another reason has been that mathematical modelling has largely been seen as an academic exercise, with ‘real’ water treatment plants designed using rule-of-thumb approaches developed with years of experience. With the emphasis on water safety, rather than economic efficiency, this approach produced conservative, working, plants.

DESCRIPTION OF AVAILABLE MODELLING ENVIRONMENTS

Five water treatment modelling packages were identified and reviewed:

- OTTER - WRc
- Stimela – TU Delft
- METREX – TU Duisberg

- WatPro - Hydromantis
- WTP – US EPA

OTTER

OTTER is a PC-based modelling package designed to dynamically simulate the performance of water treatment works (Head *et al*., 2002). Development of OTTER as a combined package began around 1996, with the earliest part of OTTER (the carbonate chemistry module) dating back to the early- to mid-1980s. OTTER development has continued since, with the last public release of OTTER in 2003. OTTER has seen use throughout the world, but predominantly in the UK and USA.

OTTER can be used to simulate individual treatment processes or a complete treatment plant (see Figure 1). The program enables process scientists and plant operators to optimise the response of the works to changes in the raw water quality, plant throughput or process operating conditions. Typical uses of the software include operational decision support, works optimisation, plant design and operator training. Version 2 of OTTER includes:

- Chemical floc formation and pH adjustment
- Clarification (floc blanket clarifiers, dissolved air flotation, sedimentation tanks, lamella settlers)
- Rapid gravity filtration
- Granular activated carbon adsorption
- Ozonation
- Disinfection
- Sludge treatment

OTTER models the occurrence, formation and removal of a wide range of water quality parameters, from general parameters such as turbidity and colour, organic parameters such as DOC, inorganics such as bromate through to pesticides and microbiological indices.

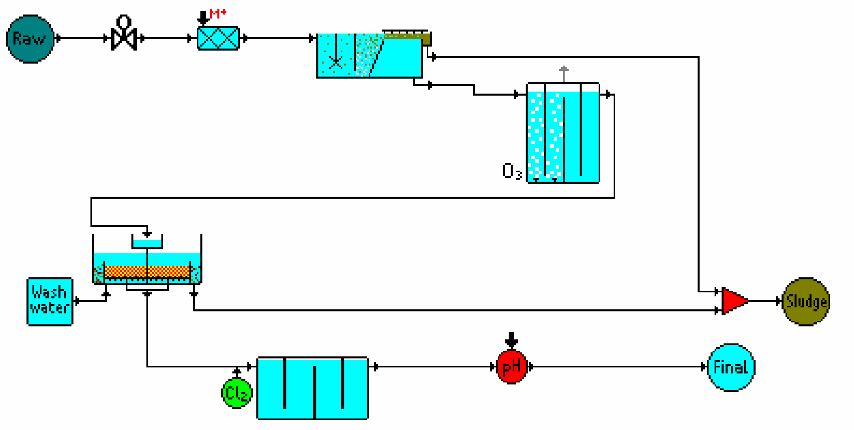

Figure 1 OTTER flowsheet

Several studies have been carried out using OTTER at waterworks (Butler, 1998; Gallis, 1999; Giraudet, 2002a, b; Guo and Sankararamkrishnan, 2003). Generally these have all been successful, but have highlighted the relatively large data requirements for successful calibration and use. The empirical nature of the coagulation and flocculation models has meant that the calibrated models could not be applied much outside the calibration region, restricting the degree of optimisation that could be studied.

Stimela

Stimela is an environment where different drinking water treatment processes can be modelled dynamically. The models of individual processes are situated in a model library and can be connected to each other, forming a complete treatment train (see Figure 2). In this way, the effect of operational changes in preceding treatment processes can be evaluated (Helm and Rietveld, 2002).

Stimela includes the following processes:

- Aeration (cascades, towers, plates, sprayers)
- Filtration (single layer, double layer, continuous, biological)
- Granular activated carbon filtration
- Softening and conditioning
- Ozonation (bubble column and contact chambers)

Stimela models dissolved compounds such as gasses (CH_4, CO_2, O_2, O_3), inorganic compounds (HCO_3^- ,NH_4^+, CO_3^{2-}, Ca^{2+}) and organic compounds (DOC, organic micropollutants, UV_{254}, AOC). In addition, floc removal is modelled by filtration.

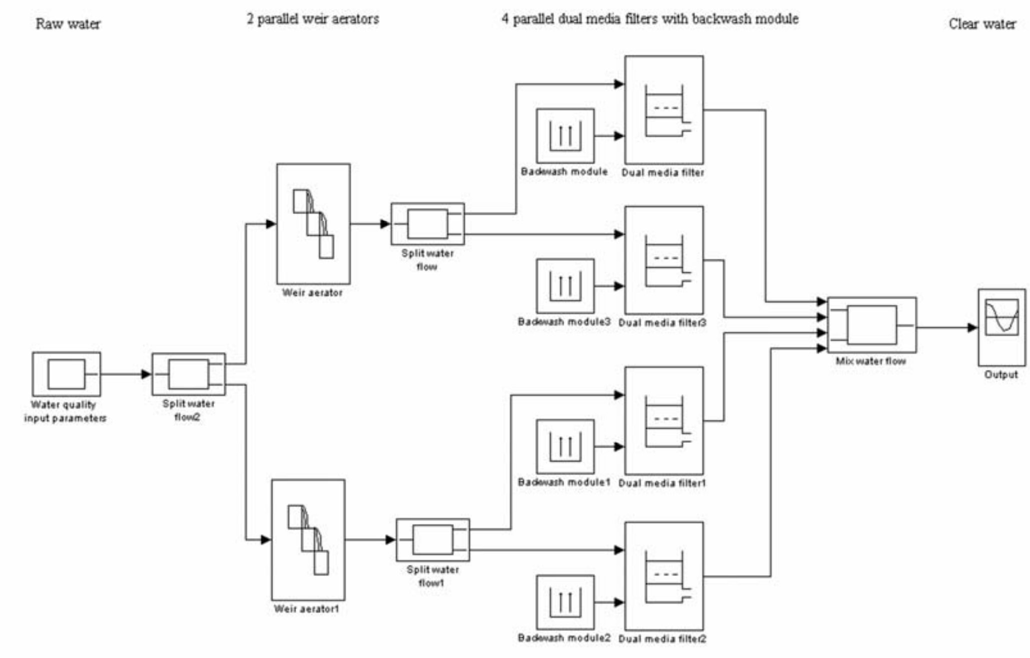

Figure 2 Example of a treatment train in the Stimela environment

The flowsheet model can be run after specifying all parameters, choosing the integration method, the step size and the simulation time. After simulation, graphical output is obtained by opening the output block. The calculated values can be compared with measured data. Typically, the output consists of water quality parameters that are relevant for the process and other data that describe the state of the process, such as filter head loss, degree of saturation of activated carbon, grain size of pellets in a softening reactor, etc.

Stimela is available on the web, at www.stimela.com, where it may be freely accessed.

Metrex

Metrex was developed at the University of Duisburg, Germany (Mälzer and Nahrstedt, 2002). It combines analytical and numerical models of common treatment steps used in surface water treatment:

- Microstraining
- Ozonation
- Floc formation
- Sedimentation
- Rapid filtration
- Granular activated carbon filtration
- Biodegradation
- Disinfection

The emphasis is on particle removal (particle size distributions are considered) and ozonation (oxidation of dissolved organic carbon, iron and manganese, and formation of bromate). Simulated plants can be configured in any combination of treatment steps. A graphical user interface assists with setting up the underlying mathematical models and required data.

Two levels of simulation exist. The first is designed to simulate the whole treatment process in operation mode, while the second provides support in designing and dimensioning single process steps. Determinands are characterized by their concentrations and in some cases additionally by their treatability (e.g. biodegradability or adsorbability on activated carbon). The models used for the simulation tools of the treatment steps are mechanistic ones. In many cases, qualitative knowledge exists about the range of values of the parameters and their dependencies on other known variables. This enables the user to estimate values for parameters by fuzzy-linguistic modelling.

WTP model

The Water Treatment Plant (WTP) model was originally developed by the United States Environmental Protection Agency (US EPA), in support of the Disinfectant/Disinfection By-products (D/DBP) Rule (Harrington *et al*., 1992). The model describes the processes:

- Coagulation/flocculation
- Settling
- Filtration
- Granular activated carbon filtration
- Softening

- Membrane filtration
- Chlorination

WTP is based on empirical relations obtained from regression analysis. It was prepared with the understanding that the predictions should reflect typical average performance values, and is focussed on the removal of natural organic matter (NOM), the formation of DBPs and disinfection. It is not to be construed that the results from the model will necessarily be applicable to individual raw water quality and water treatment at specific municipalities. This model does not replace sound engineering judgement based on site-specific treatability data to evaluate the best manner in which to address the requirements of the Surface Water Treatment Rule (SWTR) or potential D/DBP Rule. It is understood that one limitation of the model is the extent of the database availability to verify model predictions. In a desire to systematically improve the overall predictive capability, the intent of the model is to solicit public comment on the usefulness and relative accuracy of the predictions on a case-by-case basis. The WTP model includes a method to enter laboratory analysis so that a comparison can be made to the model predictions. In 2000, the WTP model was modified. Old algorithms were updated and new process algorithms were added, especially related to inactivation of microorganisms, formation of DBPs and the decay of disinfectants.

WatPro

WatPro is supplied by Hydromantis Inc. It is a steady-state water treatment modelling 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. The information in this section is taken from the WatPro User Guide (Hydromantis, 2004).

Supported treatment processes are:

- Flocculation;
- Settling basin – this model does not appear to do any specific settlement; rather, the user specifies the outlet turbidity;
- Filtration – simple models, where the user specifies the percentage removal of TOC and UV_{254}, and optionally the effluent turbidity;
- GAC adsorption – this appears to be an incomplete model, as it uses a Freundlich isotherm to describe removal of TOC and UV_{254} but requires that the user provide only one of the two parameters in the Freundlich model, the exponent n;
- Membrane treatment – again a simple model, where the user specifies the percentage of water produced through the membrane (the remainder is treated as the waste stream, i.e. the concentrate) and optionally the effluent turbidity;
- Contact tank – for chlorine disinfection;
- Ozonation – ozone disinfection.

WatPro's strength is in the prediction of chlorination by-products, using published US EPA correlations. It is less useful in modelling other aspects of water treatment, as all other water treatment processes are defined by the user specifying either a percentage removal - which is independent of water quality or flow - or an outlet turbidity from the process tank - again independent of water quality or flow.

EVALUATION

Each of the water treatment modelling packages discussed above has its specific characteristics. OTTER contains models for most commonly encountered processes and less conventional processes may require development of a suitable mathematical model (Butt and Head, 2002).

The main purpose of Stimela is to support research and development, and control applications. Therefore, it focuses on model development, programming is open and structured and graphical output is flexible.

Metrex was developed mainly to examine the use of particle size distribution as a modelling approach to better understand particle removal processes, rather than general water treatment. Metrex is not actively being developed.

The WTP model was developed to simulate the general case rather than the site-specific case. Some drinking water treatment plant operators may be tempted to use this model as a substitute for site-specific studies. However, the output from the model is not intended to, nor should it, replace sound engineering judgement based on bench-, pilot- and field-scale treatability studies for specific waters (Harrington *et al*., 1992). The model is mainly used for evaluation of design rather than operational optimisation studies.

CONCLUSIONS

1. Although flowsheeting programs have been applied to water treatment modelling since the 1990s, available software packages have not been widely adopted by the water industry.

2. Five water treatment modelling packages were reviewed; each had its strengths and weaknesses.

3. OTTER and Stimela were selected as the basis of the framework for the new water treatment simulator to be developed as part of TECHNEAU.

4. Work is now underway to integrate the two existing models and to design the modelling framework.

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