

Water treatment simulators

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ABSTRACT

The EU-funded project, TECHNEAU, is intended (among other tasks) to develop a new water treatment simulator, in part to implement new process models to be developed within TECHNEAU. Before beginning any software development there has been a review of existing water treatment simulators, to identify what would be needed for a 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.

Key words | flowsheeting, process modelling, water treatment

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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 linked 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. A third reason has been the expectations raised about modelling. Because water is seen as clean and well-characterised there has been an expectation among some users that the models should be highly accurate. Where a model could help in determining

pass/fail performance envelopes this was regarded as insufficiently accurate, because it required engineering judgement in determining the boundary between pass and fail performance. However, other users have accepted that modelling, however complicated, still represents an idealisation of the physical processes and therefore expected the models to provide insight and engineering support. These users usually found modelling support more productive.

PROCESS FLOWSHEETING

While water treatment works modelling appears to be a specific research area, it can be regarded as simply a specialisation of process flowsheeting. That is, there is a specific set of unit process models appropriate for water treatment, but the underlying structure is the same whether the flowsheet comprises water treatment, wastewater treatment, or chemical process industry unit process models; there is a treatment train involving recycles, and what is needed is an efficient solution method for the recycles, and a further efficient solution method for the whole flowsheet. This problem, process flowsheeting, has been extensively studied. There are several monographs available in the literature, of which probably the most widely quoted is

Process Flowsheeting (Westerberg et al. 1979). The main aspects of flowsheeting, excluding the process-specific models, are ordering the calculations to maximise computation speed if there are recycle loops present in the flowsheet, and detecting and handling any discontinuities in the calculations (such as a pump switching on and off).

Recycle handling

A large part of the theory of process flowsheeting is concerned with handling recycle loops. For dynamic models, recycle loops are potentially of lesser concern, depending on the solution approach chosen for the dynamic equations.

Providing the sludge train is ignored, waterworks can be regarded as having no recycle loops, and this assumption has been semi-implicit in most water treatment programs. WRC's water treatment simulator, OTTER, was extended to include the handling of waterworks sludges in the late 1990s, and at this time the effect of recycle loops became more important. If the sludge train is included, then a potential flowsheet would look like that in Figure 1, which shows one recycle. The recycled thickener supernatant flow and quality from the sludge thickener depend on the sludge produced by the DAF (dissolved air flotation), RGF (rapid gravity filters) and manganese filters, but their sludge production in turn is affected by the recycled sludge liquors from the sludge thickener.

If there are few recycles, and the fraction of flow in the recycle is small compared with that in the main liquid line, then a simple iterative process is usually sufficient to solve the recycle loops. With dynamic models, where the flows usually change by a small amount from one timestep to another, then the error may be acceptable if the iterative nature of the recycle loop is ignored, and a small time-synchronisation error is accepted for the recycle flows.

However, as the number of loops increases, or as the fraction of flow in the recycle loops increases relative to the

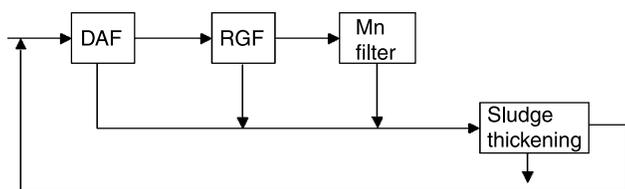


Figure 1 | Simple flowsheet.

main liquid flow, then ignoring the correct solution of the recycles may lead to an erroneous solution of the mass balance.

Even here a simple iterative solver is usually acceptable with dynamic methods, providing all the equations are solved globally. Where a sequential modular calculation process is used, such as in WRC OTTER, then more advanced loop handling is needed to accelerate the solution of the loops. There are two aspects to this acceleration. The first is to reorganise the calculation sequence so as to minimise the number of loops that must be solved; Westerberg et al. (1979) provide suitable algorithms. The second is to consider using an alternative to simple repeated substitution in the iterative solver. The most common alternative used is the Wegstein method, a form of secant method. However, limited testing on water industry applications has found that repeated substitution is still an acceptably effective solution method, and, unlike the accelerated iterative methods, does not incur a risk of numerical instability.

Dynamic modelling

There are three approaches to solving the differential equations for the process models: modular sequential, modular global and global.

Modular sequential

Each module has its differential equations integrated over the period t_{start} to t_{end} . Each downstream process is provided with the outlet streams defined at t_{start} and t_{end} , and assumes a linear variation in flows and water quality between the period t_{start} and t_{end} .

Modular global

This is similar to the global method but the differential equations are integrated on a process model basis. As an example, if each process model comprised 100 equations and there were ten process models, the modular global method calls the integration routine ten times, solving 100 equations each time, while the global method would call the integration routine once, solving 1,000 equations. For explicit integration methods, there is little difference between the two approaches, but for implicit methods there is potentially a large

improvement in computational speed and memory requirements from the modular global approach. The modular global method requires an additional piece of code to ensure that the integration timestep is set across all process models to the smallest found, to ensure that all models are synchronised as they integrate forwards in time.

Global

The global method assembles all the differential equations together and passes them to the integration routine. This provides the greatest simplicity and flexibility, at the expense of potentially larger memory requirements than the modular global method. Specifically, if a timestep is too large for any one process, the global method handles this automatically, while the modular global method requires this to be flagged up and all process models to be recalculated. On the other hand, if the timestep is too large for the first process model calculated, then there is a reduction in overhead as the remaining models would not be calculated until the timestep had been adjusted to an acceptable level for the first process.

There are many methods for solving the differential equations. For water treatment it has usually been sufficient to use the low-order Runge-Kutta method, with a stabilised Runge-Kutta-Chebyshev variant for moderate degrees of stiffness. Matlab/Simulink, the basis of the Stimela water treatment simulator, prefers to use a low-order Gear solver, as this is fairly efficient for stiff processes with mild discontinuities as may be found in typical electrical engineering problems.

Event location and handling

Events fall into two main categories: those handled as differential equations and those handled as algebraic equations.

Differential equations

A typical differential equation-based event is filling a tank, where the differential equation has a sharp change when the tank is filled (there is no further increase in volume, and any additional inflow must appear as an overflow).

Differential events are normally handled automatically by the differential equation solver, but may result in small

timesteps (and slow calculation speed) around the location of the event. If the modular sequential calculation strategy is used, then such events can cause difficulty in providing a valid solution.

Algebraic equations

A typical algebraic event is found in modelling a wet-well pump, where the pump is switched off when the level falls below a minimum value and switched on when the level rises above some set value. Between those two levels, the pump is on or off based on its history: if the level is generally rising then the pump is off, if generally falling then the pump is on. But at any instant the level may be rising and the pump may be on, if the inflow at that time exceeds the pump rate. The pump behaviour is then handled by storing whether the pump should be currently on or off between the on and off levels.

If a tank overflows during the period t_{start} to t_{end} , so that the flow in the overflow at the start was zero, and at the end some positive value, what should be the correct value to use at t_{end} ? If it is the actual flow, then downstream processes, which see only the two values at t_{start} and t_{end} , will overestimate the mass of water and water quality components. If, however, some averaging is used to ensure that the mass balance is correct (which can be done by specifying a constant flow and water quality at both t_{start} and t_{end} or choosing the values at t_{end} so that linear interpolation produces the correct integrated value), then any hydraulic impacts will be wrong (because the flow is too low). Also, water quality values will be too low for some of the period, which may result in the wrong control actions being taken; the true discontinuity may be required by downstream processes (such as scheduling backwash intervals).

Further, if the discontinuity occurred entirely within the integration interval – for example, the tank has an overflow that occurs after t_{start} but has ended before t_{end} – what then should be the correct values in the overflow stream? Should the mass balance be conserved, or should greater emphasis be given to the observation that the flow in the overflow stream as measured would be zero at both t_{start} and t_{end} ?

For these reasons the use of modular global, or global, solution methods are to be preferred. WRC's OTTER program uses the modular sequential solution strategy, and users are warned that they may need to use a tiny

output timestep if they think that such discontinuities are affecting the accuracy of the simulation. This means that the timestep is always small, to catch the discontinuity.

DESCRIPTION OF AVAILABLE MODELLING ENVIRONMENTS

There are currently five main water treatment modelling packages available. These are:

- OTTER (WRc)
- Stimela (TU Delft)
- Metrex (TU Duisberg)
- WTP (US EPA)
- WatPro (Hydromantis)

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. The focus of the program has been the practising engineer, rather than the research community.

The program can be used to simulate individual treatment processes or the whole treatment plant (see Figure 2). It 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 (GAC) adsorption
- Ozonation
- Disinfection
- Sludge treatment

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

The solution approach is modular sequential. OTTER also includes a loop detector. Many dynamic sequential modular systems cannot adequately handle recycles, because the solution approach requires either that each recycle is in error, for the flow terms, by one timestep, or that a computationally expensive iterative procedure be used. OTTER attempts to side-step this by ordering the calculations as much as possible to split recycles and keep the outputs in phase in time. OTTER further includes the option to iterate around each loop, typically with up to five iterations before abandoning attempts to iterate further to full convergence.

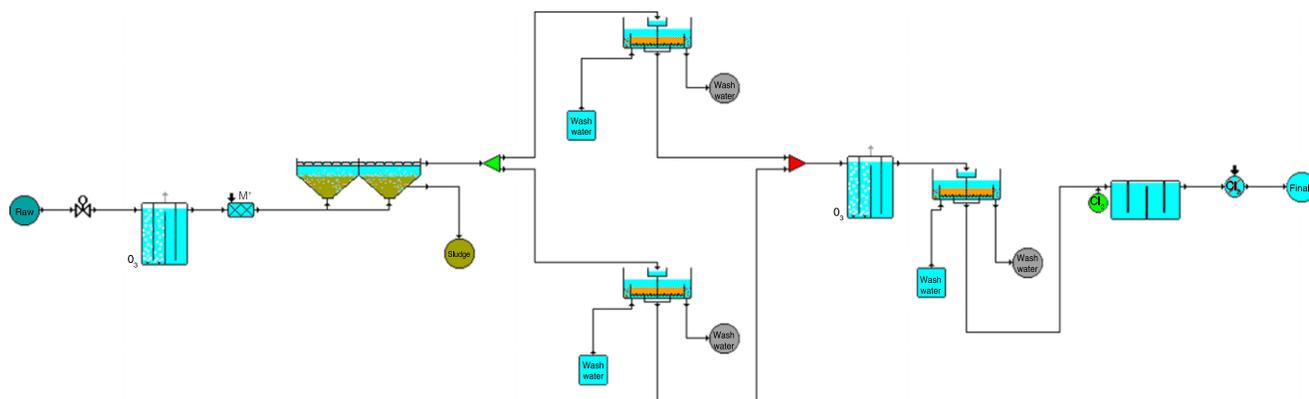


Figure 2 | OTTER flowsheet.

Several studies have been done using OTTER at waterworks (Butler 1998; Gallis 1999; Guo & Sankaramakrishnan 2003). Generally these have all been successful, but have highlighted the relatively extensive 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 with great confidence outside the calibration region, restricting the degree of optimisation that could be studied.

Stimela

Stimela is an environment in which 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 3). In this way, the effect of operational changes in preceding treatment processes can be evaluated (van der Helm & Rietveld 2002). Stimela is the only program that attempts to cover both the practising engineer – as a tool for use mainly by

the Dutch company DHV – and the research community. This has affected Stimela's ease of use, as the requirement to make it easy to add new models has encouraged the use of the MATLAB/Simulink environment. Because Matlab/Simulink is used, the models are easily accessible, the structure is open and flexible and all routines, toolboxes and visualisation techniques of Matlab/Simulink can be used (van der Helm & Rietveld 2002). However, this does require that end-users purchase a copy of Matlab/Simulink, and for non-academic users the purchase cost is high. Simulink has many strengths, but its mental model is centred on the electrical engineering and process control community, making it less accessible to civil and water engineers. Like all programs, such a barrier does not affect regular users, but does inhibit less frequent users.

Stimela includes the following processes:

- Aeration (cascades, towers, plates, sprayers)
- Filtration (single layer, double layer, continuous, biological)
- Granular activated carbon filtration

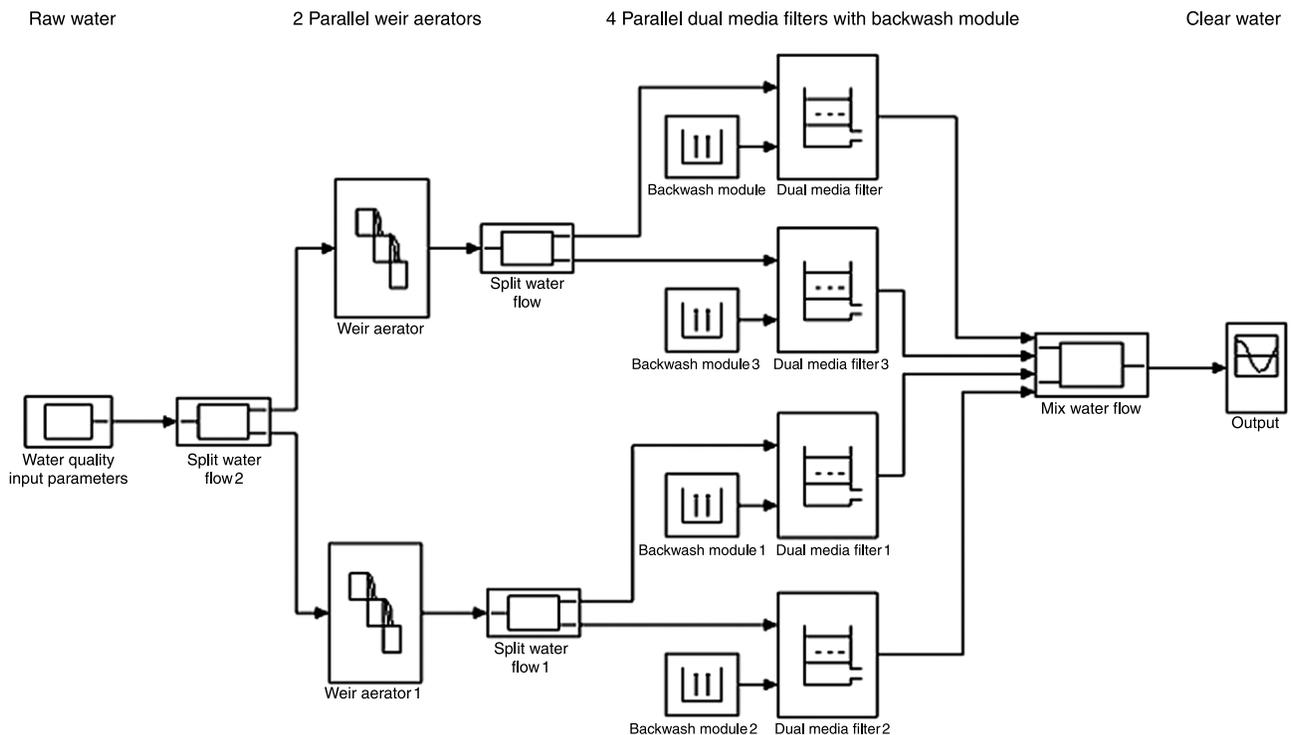


Figure 3 | Example of a treatment train in the Stimela environment.

- Softening and conditioning
- Ozonation (bubble column and contact chambers)

Stimela models the fate of dissolved gases (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 [assimilable organic carbon]). In addition floc removal is modelled by filtration.

After specifying all parameters the flowsheet model can be run, 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, and so on.

Stimela is available on the Internet, at www.stimela.com, where it may be freely accessed. The web-based interface does not exploit the full power of Stimela, as it makes use of a small selection of flowsheets. More general use is available, but this requires running each process model in isolation, with 'copy and paste' to transfer data between the different process models.

METREX

Metrex was developed at the University of Duisburg, Germany (Mälzer & Nahrstedt 2002). Metrex was developed as a research tool rather than for general engineering use. Like Stimela, Metrex was built on the MATLAB/Simulink platform. However, unlike Stimela, Metrex has been made available with a simple interface that does not expose the MATLAB/Simulink environment. This has reduced its flexibility compared with Stimela. MATLAB/Simulink must still be purchased by the end-user because Metrex still calls on the MATLAB and Simulink libraries.

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, formation of bromate). Simulated plants can be configured in any combination of treatment steps. A graphical user interface (GUI) 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 characterised by their concentrations and in some cases additionally by their treatability (e.g. biodegradability, adsorbability on activated carbon, etc.). 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 dependences 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). As such, the program is firmly focused on the practising engineer, and is intended only to calculate the disinfection effects of the various treatment processes. The following processes are included in the program:

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

The WTP model 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 focused 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 treatment effects at specific treatment works. 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 an attempt 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 with 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 (Hydromantis 2004). Like WTP, it is aimed at the practising engineer, and appears to be an extension to WTP to include more effects of water treatment processes than just disinfection. However, these other aspects of water treatment processes are of lesser significance within the package's scope.

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 (total organic carbon) and UV_{254} , and optionally the effluent turbidity
- GAC adsorption – this appears to be a simplified 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 either specifying 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 plant models discussed above has its specific characteristics, summarised in Table 1.

OTTER contains models for most commonly encountered processes while less conventional processes may require development of a suitable mathematical model (Butt & Head 2002). The models provided with OTTER cover those typically needed in the UK and USA, but exclude other processes more common elsewhere in Europe, such as water softening. There is a facility to add new process models but it is not well documented, nor is it as easy and flexible as the method adopted by Stimela. OTTER was found to be easy to use, as was WatPro, because of its use of a GUI-based 'drag & drop' flow-sheeting environment. This environment is now largely standard, found in the wastewater treatment simulators, the chemical process and oil and gas simulators, and in other (non-process modelling) flowcharting environments such as Microsoft's Visio program.

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. Stimela is geared towards the needs of the Dutch water industry, so that while it has good models for water softening it ignores many of the solids/turbidity removal processes. Because of Stimela's adoption of MATLAB/Simulink as the modelling platform it is easy to add

Table 1 | 1 Summary characteristics of available programs

	OTTER	Stimela	Metrex	WTP	WatPro
Dynamic?	Y	Y	Y	N	N
Sludge processes?	Y	N	N	N	N
Recycles?	Y	Y	N	N	N
Disinfection models?	Y	Y	Y	Y	Y
Clarification?	Y	N	Y	N	N
Filtration?	Y	Y	Y	N	N
Easily extendible?	N	Y	N	N	N
Engineering use?	Y	Y	N	Y	Y
Research use?	N	Y	Y	N	N
Easy to use?	Y	N	N	Y	Y
Readily redistributable?	Y	N	N	Y	Y
Solver method	Modular sequential	Global	Global	Modular sequential	Modular sequential

new process models, using a mixture of MATLAB and Simulink code. The resulting process models operate in a semi-interpreted environment and therefore the simulations are slower than the programs using fully-compiled languages (OTTER, WTP and WatPro).

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 currently under development, following the completion of the research programme, and is not readily available. Although Metrex is based on MATLAB/Simulink, like Stimela, it was found to be difficult to use, even by experienced Stimela users.

The WTP model was developed to simulate general water treatment 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.

WatPro does not appear to offer any real benefits over WTP. Its disinfection models are taken from those used in

WTP, while its models for solids and turbidity removal are simple percentage removals, or constant values, specified by the user. There is no attempt to relate turbidity/solids removal to any operational aspects, such as loading rates. WatPro is therefore inappropriate for providing any insight into water works operation.

TECHNEAU SIMULATOR

One of the aims of the EU-funded TECHNEAU project is to produce a new-generation water treatment simulator. This will build on the experiences of OTTER, Stimela and Metrex, reusing process models from these programs wherever possible. One part of the TECHNEAU project will also look at developing new process models for processes where either there are no existing models or the existing models require improvement. Coagulation/flocculation is one such model. The GUI of the TECHNEAU simulator will be based on the OTTER interface, with Stimela providing mechanisms to add new models. The TECHNEAU water treatment simulator will be made freely available via the Internet.

The technical aims of the new simulator include the following:

- Overall mass balance (water recovery, side streams)
- Effect on microbial composition (inactivation or removal of protozoan cysts/oocysts, bacteria/spores and viruses), i.e. barrier effect
- Effect on chemical speciation (e.g. alkalinity, pH, coagulant residual, calcium, magnesium, iron, manganese, bromide, ammonia)
- Effect on colligative properties (e.g. TOC, UV-absorbance, colour, turbidity)
- Process dependence of downstream or upstream processes and consequences on performance

The program will be tested initially at five water treatment works owned by TECHNEAU partners or end-users, spread across the EU. The supported process models for the initial release will therefore include most treatment processes found at large waterworks within the EU, rather than just in the UK or the Netherlands. There will be a greater focus on providing calibration support, and on working with the waterworks to minimise the cost of acquiring calibration data.

Experience with OTTER and Stimela has indicated that water companies are prepared to acquire extensive and non-routine data for model calibration, providing that the resulting model produces predictions of usable accuracy, and can be applied outside the calibration envelope. Many Dutch waterworks have online particle size monitors; few UK waterworks have this level of instrumentation. However, if the Metrex-style approach to modelling using particle size distribution data is shown to be of value in improving operational performance and cost, then water companies will be willing to make such an investment. One benefit of testing the program across several countries is that better-instrumented waterworks can be used to demonstrate whether data-intensive models will reward the data collection effort.

CONCLUSIONS

The current generation of water treatment simulators are, in the main, acceptable for process modelling. There are two main shortcomings:

- The coagulation/flocculation process, where the models are too empirical, too data intensive, and have a limited applicability range outside the calibration area
- The data requirements for effective calibration; the current data needs cause problems with unfamiliar determinands and the high frequency of measurements

The TECHNEAU project intends to develop a new-generation simulator which will address these two issues, and build on the successes embodied in the OTTER, Stimela and METREX programs.

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