



Models for Drinking Water Treatment

Review State-of-the-Art

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1 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 (Wistrom and Farrel, 1998; Zang and Stanley, 1999; Baxter, 1999; Yu et al., 2000; Baxter et al., 2001; 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 were introduced in the chemical industry in the 1960s, and in wastewater treatment in the 1970s, but it was not until the 1990s that it was 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 activity, with 'real' water treatment plants designed using rule-of-thumb approaches by engineers with years of experience. With the emphasis on water quality, rather than economic efficiency, this approach produced working, if somewhat conservative, plants.

With growing pressures on water treatment there is now a greater need to optimise water works, whether to increase throughput, reduce operational costs, or minimise capital expenditure. One tool that can assist with this is water-treatment flowsheeting packages. Although programs for individual treatment processes, of various quality and in different programming languages, exist there are only a few packages for the simulation of the entire treatment plant. This report focuses on the State-of-the-Art of these modelling platforms for drinking water treatment. The programs that are considered are known from the literature, found through Internet searches or obtained by informal contacts.

2 Description of Modelling Environments

The following drinking water treatment modelling platforms are selected for description and evaluation:

- OTTER, from WRc, a project partner and for which full source code is available
- Stimela, from TU Delft, a project partner and again for which full source code is available
- METREX, from Duisburg University. Although not a project partner they are collaborating through TU Delft and have agreed to make available their source code.

The following programs are also discussed, although source code for these programs is not available:

- WatPro
- WTP
- TAPWAT

2.1 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 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 program can be used to simulate individual treatment processes or the whole treatment plant. 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 adsorption
- Ozonation
- Disinfection
- Sludge treatment

OTTER models the formation and removal of a wide range of water quality parameters, including general parameters such as turbidity and colour, organic parameters such as DOC, inorganics such as bromate, pesticides and microbiological indices. A full list can be found in Annex I.

OTTER supports user-added models using a dynamic link library. Thus many programming languages can be used to develop new OTTER models, additional to those provided in the basic suite, reducing the effects of 'vendor

lock-in' compared to simulation packages that use proprietary languages. However, the experience of WRc has been that few users have the skill, experience or interest to develop models of their own, preferring instead that such models as they need be developed for them and included in the core OTTER system.

OTTER itself is written in a combination of Microsoft's Visual Basic, for the user interface, and Fortran code, for the numerical models. The Fortran code has demonstrated its adaptability, as different Fortran compilers have been used during OTTER's history. The Visual Basic code is, of course, tightly coupled to Microsoft and only available through Microsoft. However, for the end user there is no need to pay for copies of Visual Basic or Fortran. An example of the visual interface is shown in Figure 2.1.

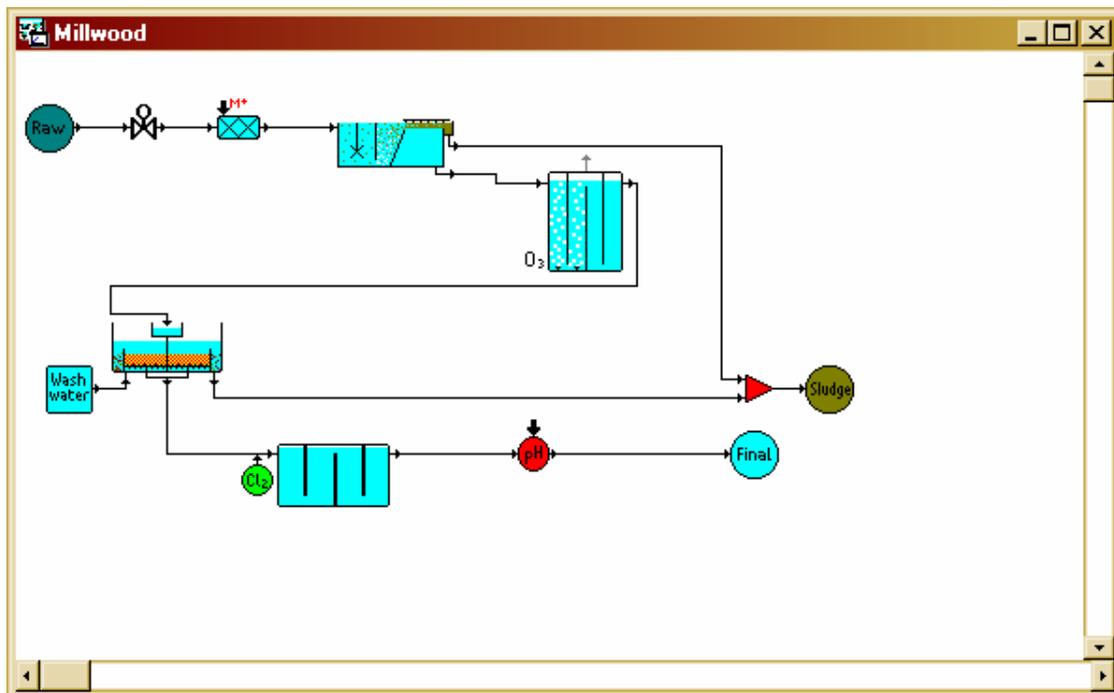


Figure 2.1 OTTER flowsheet

The solution approach is modular sequential. That is, at each timestep, all the differential equations in a process unit are integrated across the range T to $T + \Delta T$. Then the next unit downstream is solved, being passed as its water flow and quality the value for the upstream process at T , treated as piece-wise constant across the integration interval. Because of this modular sequential solution method a loop finder, with reordering of the calculation order to minimise the effects of loops, and iteration around the loops, is automatically provided. The calculation order can be altered by the user.

Several studies have been done 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.

2.2 Stimela

Stimela is an environment where different drinking water treatment processes can dynamically be modelled. The Stimela models are developed in Matlab/Simulink. Matlab is a commercial modelling environment available from The MathWorks. It comprises a language geared around matrix methods and is extensively used in academia and as a prototyping environment. There are many add-ons to Matlab to simplify its use in a wide number of areas – The MathWorks claim that there are several hundred commercial toolboxes available. The most widely used toolbox is the simulation toolbox, Simulink. Matlab/Simulink has been used by both Metrex and Stimela, and has also been used by a wastewater modelling environment, Simba, which was the inspiration for Stimela and Metrex electing to use Matlab/Simulink.

Partial differential equations are converted into ordinary differential equations, usually by using either finite differences or a series of mixed tanks. The resulting ordinary differential equations are numerically integrated so that variations in time and space can be followed. 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 2.2). In this way, the effect of operational changes in preceding treatment processes can be evaluated. 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 (Helm and 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. In addition, the use of Matlab/Simulink results in a user interface that is more difficult to learn than more customised simulation software.

Stimela includes the following processes:

- Aeration (cascades, towers, plates, spayers)
- 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 by filtration is modelled. A full list is available in Annex I.

A Stimela model consists of a raw water block, followed by one or more process blocks, control blocks and graphical output blocks. The raw water can be specified as constant values, or a datafile can be specified to provide time-varying values. The connecting line between blocks transfers the values of the water quality parameters at every time step. By opening the process block, design, and calibration parameters can be inserted. The design parameters (e.g. tank volume) are fixed. Calibration parameters are water-specific and must be obtained through experiments. Calibration is executed with obtained measurement data of a pilot or full-scale plant. Calibration parameters can be floc density, filtration coefficients, Freundlich- constants, gas transfer coefficient, etc. Control blocks can be used to further manipulate the process blocks, varying calibration or operational parameters.

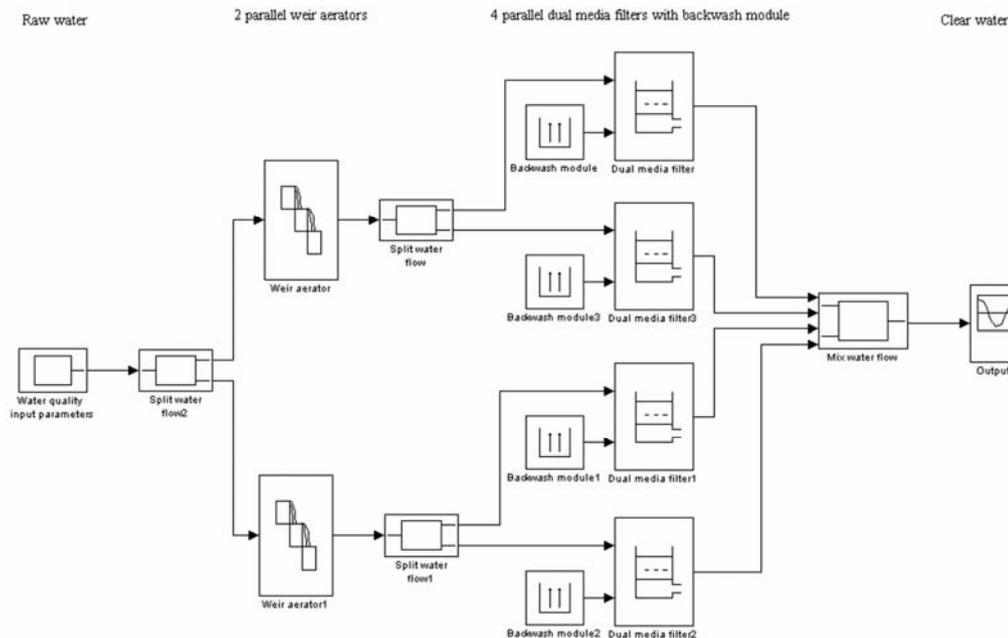


Figure 2.2 Example of a treatment train in the Stimela environment

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

2.3 Metrex

Metrex was developed at the University of Duisburg, Germany (Mälzer and Nahrstedt, 2002). The simulation tools combine 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 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. The software concept is based on an object-oriented model using Java technology, World-Wide-Web (WWW) browsers and the simulation software tool Matlab/ Simulink. Each process step is designed with a uniform structure. Water compounds are characterized by their concentrations and in some cases additionally by their treatability (e.g. biodegradability, adsorbability on activated carbon). Reports of the simulation results, including all water parameters, are generated automatically in Hyper-Text-Mark-up-Language (HTML) format. Documentation is also given using HTML files. Mechanistic models are used. 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 using fuzzy-linguistic modelling.

2.4 WTP model

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

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

It 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 treatment effects 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. Existing algorithms were updated and new process algorithms were added, especially related to inactivation of microorganisms, formation of DBPs and the decay of disinfectants.

2.5 TAPWAT

TAPWAT (Tool for the Analysis of the Production of drinking WATER) was 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 risk levels by micro-organisms) given a certain raw water quality
- To determine the probability of occurrence of pathogenic microorganisms and DBPs in the product of a treatment plant
- To advise the drinking water inspectorate by reviewing new or renewed production plants especially concerning public health risks

The program supports percentage-removal based, empirical and mechanistic models for all process units. The choice as to which level of complexity to use is then made based on available data and user confidence with mechanistic models outside their calibration region. The program was developed according to RIVM standards for information infrastructure and modelling (Versteegh et al., 2001).

Percentage removal models were developed using information from the open literature, reports, data from production plants and expert judgement to provide design ranges of percentages for removal of microorganisms and compounds by the selected treatment processes.

Process models for the formation of DBPs by chlorination and ozonation were tested using data from full-scale plants in the Netherlands.

The beta-distribution is used for statistical analysis of data of production plants, especially for the removal of TOC and turbidity by floc formation, floc removal and activated carbon filtration. The distribution of the product water quality parameters is determined by the distribution of the influent water quality parameters and the distribution of the removal percentages. For this, Monte Carlo techniques are used.

2.6 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:

- Measurement point: This is used to adjust the water quality at any point to measured values. It is specifically intended to allow raw water quality to be adjusted to reflect any unmodelled treatment processes, or correct for any deficiencies in the model output compared to experience
- Flocculation
- Settling basin – this process does not appear to model settlement; rather, allowing the user to specify the outlet turbidity
- Filtration – simple models, where the user specifies the percentage removal of TOC and UV254, and optionally the effluent turbidity

- GAC – this appears to be an incomplete model, as it uses a Freundlich isotherm to describe removal of TOC and UV254 but requires that the user provide only one of the two parameters in the Freundlich model, the exponent n
- Membrane – again a simple model, where the user specifies the percentage of water produced through the membrane (the remainder (the waste stream) is treated as 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 otherwise a poor example of the state of the art in water treatment, modelling all other water treatment processes by the user either specifying a percentage removal, which is independent of water quality or flow, or an outlet turbidity from the process, again independent of water quality or flow. Because of these serious deficiencies the use of WatPro for any purpose other than modelling disinfection should be avoided by inexperienced users.

3 Determinands

The appropriate selection of determinands (water quality parameters) in water treatment should ideally meet the following criteria:

- Be based around what is likely to be measured, and not over-whelm the user with a large number of unnecessary determinands
- Have the ability to add new determinands, as water quality requirements change – for example, it is likely that modelling the fate of endocrine-disrupting chemicals may be of greater interest in future
- Provide a comprehensive list of determinands, so that the user does not have to locate any needed physical or chemical property data

Clearly these requirements impose some conflicts. For OTTER, Stimela and METREX an overview of the determinands is given in Annex I.

The OTTER approach has been to provide a large, but organised, list of all determinands that can be modelled. The addition of any new determinands would potentially require modifications to all unit processes. The OTTER determinands dialogue screen is shown in Figure 3.1.

The screenshot shows a software window titled "Water quality profile [Upland seasonal]". It features a menu bar with options: General, Total Metals, Dissolved Metals, Inorganics, Organics, Pesticides, Microbiological, and Others. Below the menu is a table with 12 rows representing months from January to December 1997. The columns are: Date/time, Time of year, pH, Temperature, Turbidity, Apparent Colour (*Hazen), True Colour, Hardness, Alkalinity, Conductivity, and Total Solids. At the bottom of the window are buttons for OK, Cancel, Reset, and Help.

	Date/time	Time of year	pH	Temperature	Turbidity	Apparent Colour (*Hazen)	True Colour	Hardness	Alkalinity	Conductivity	Total Solids
1	01.01/1997 00:00	01 Jan 00:00	5.00	6.00	1.10	27.00	23.00	23.00	14.00	50.00	
2	01.02/1997 00:00	01 Feb 00:00	5.40	8.00	1.30	20.00	15.00	22.00	14.00	48.00	
3	01.03/1997 00:00	01 Mar 00:00	5.50	9.00	1.40	23.00	17.00	21.00	13.00	45.00	
4	01.04/1997 00:00	01 Apr 00:00	5.80	10.30	1.40	24.00	18.00	22.00	13.00	45.00	
5	01.05/1997 00:00	01 May 00:00	5.60	13.20	0.80	21.00	18.00	19.00	14.00	49.00	
6	01.06/1997 00:00	01 Jun 00:00	5.50	16.90	0.40	30.00	28.00	19.00	11.00	39.00	
7	01.07/1997 00:00	01 Jul 00:00	5.50	18.00	0.80	38.00	35.00	20.00	10.00	34.00	
8	01.08/1997 00:00	01 Aug 00:00	5.70	16.80	1.00	30.00	26.00	20.00	11.00	38.00	
9	01.09/1997 00:00	01 Sep 00:00	5.40	17.00	1.40	39.00	33.00	19.00	10.00	35.00	
10	01.10/1997 00:00	01 Oct 00:00	5.60	17.00	1.20	33.00	28.00	21.00	10.00	36.00	
11	01.11/1997 00:00	01 Nov 00:00	5.50	16.80	1.20	30.00	25.00	24.00	11.00	37.00	
12	01.12/1997 00:00	01 Dec 00:00	5.00	9.00	1.00	29.00	25.00	23.00	14.00	49.00	

Figure 3.1 OTTER determinands

Stimela, on the other hand, provides a smaller list of determinands, and allows the user to make active only those parameters that are actually required. However, there is less emphasis on trying to categorise the determinands. The Stimela determinands dialogue menu is shown in Figure 3.2.

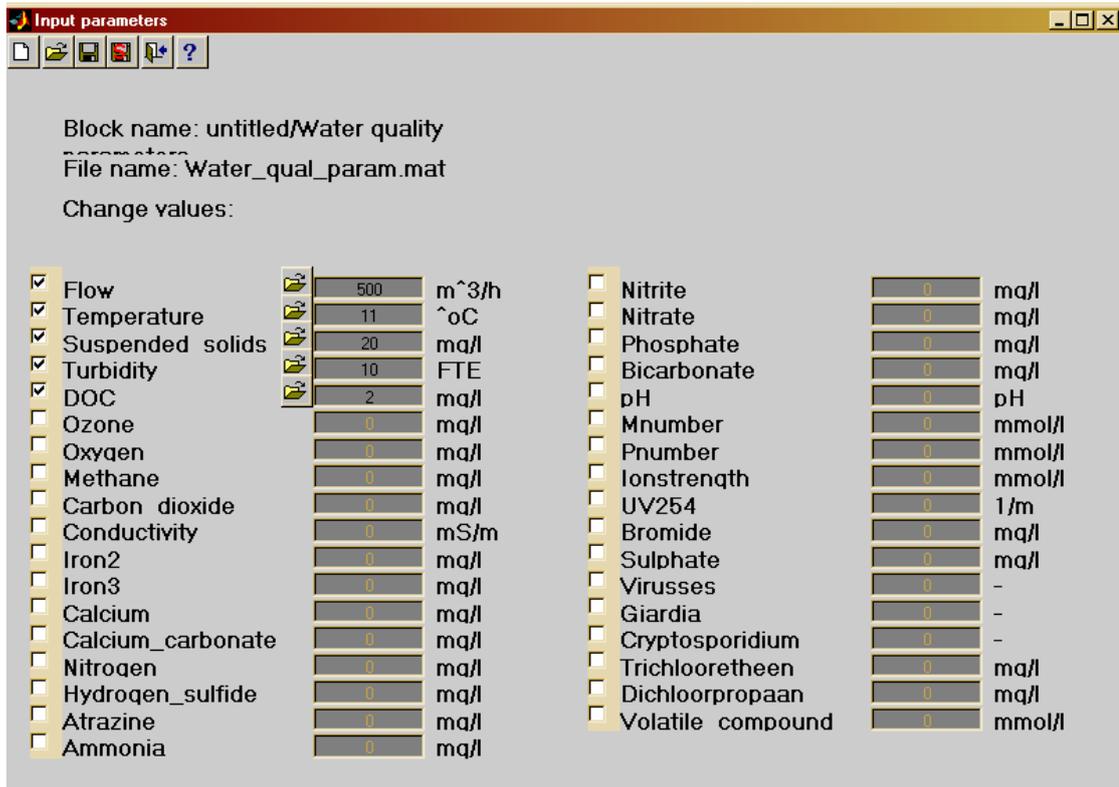


Figure 3.2 Stimela determinand dialogue

Metrex also categorises the determinands. Its initial determinand dialogue is shown in Figure 3.3



Figure 3.3 Metrex determinand dialogue

4 Evaluation

Each of the water treatment plant models 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). OTTER is a well-developed model for design purposes in particular. It is graphically good and it is easy to build up a treatment plant. Visualisation and calculations are separated. It is well documented and models of many different conventional treatment steps are available. The main weak point is that it is a compiled program and therefore it is difficult for general users to add new process models.

Stimela uses Matlab for its calculations and can also use its functionalities (integrator, loop detector, debugging). Stimela has a Web interface, but it is limited to single processes. 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. Although documentation is limited several scientific publications (journals, congress proceedings, PhD thesis) are available describing the results of the modelling efforts. Operating within Matlab/Simulink, many of the models are interpreted and simulating large systems the simulations can require extensive calculation time. It is also difficult for general users to add new process models without an extensive knowledge of Matlab/Simulink and the Stimela framework, plus, of course, licenced copies of Matlab and Simulink.

Metrex is being developed mainly for particle removal, but has as an advantage that it is written in an accessible language and exchange and development is easy. Metrex, like Stimela, makes use of Matlab. Simulation on different levels is possible and many different water quality parameters (determinands) can be incorporated, but not all in use. However, Metrex is currently moribund.

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). In fact, the model is mainly used for evaluation of design rather than operational optimisation studies.

With TAPWAT stochastic and simple process modelling can be performed for pathogenic microorganism removal and disinfection by-product formation. The model is not intensively tested and still in a development phase. It is not used outside RIVM.

WatPro is effectively a generalisation of WTP, and its algorithms replicate those found in WTP and the disinfection modules of OTTER and Stimela.

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Annex I: Determinands of different programs

Otter	Stimela	Metrex
General: pH, Temperature, Turbidity, colour, Total hardness, Alkalinity, EC, TSS, SSS, FSS, Cl, ClO ₃ , ClO ₄	pH, Temperature, Turbidity, Total hardness, Alkalinity, EC, TSS	Ph, Ks, Kb, alkalinity
Metals: Al, Mn, Fe	Fe	Al, Mn, Fe
D.O. (mg/l)	Gasses: CO ₂ , O ₂ , O ₃ , CH ₄	O ₂ , O ₃ , N ₂
Inorganics: Ammonia (mg/l), Nitrate (mg/l), Nitrite (mg/l), Chloride (mg/l), Chlorite (mg/l), Chlorate (mg/l), Bromide (µg/l), Bromate (µg/l), Sulphate (mg/l), Orthophosphate (mgP/l)	NH ₄ , NO ₂ , NO ₃ , PO ₄	BrO ₃ , Br, Ca, Cl, F, K, Mg, NH ₄ , NO ₂ , NO ₃ , OH, PO ₄ , SO ₄ , HCO ₃ , CO ₃
Organics: TOC (mg/l), DOC (mg/l), POC (mg/l), THMs (µg/l), THMFP (µg/l), HAAs (µg/l), AOC (µg/l)	DOC, TOC, UV ₂₅₄ , AOC	DOC, UV ₂₅₄ , UV ₄₃₆
Pesticides: Simazine (µg/l), Chlortoluron (µg/l), Diuron (µg/l), Isoproturon (µg/l), MCPA (µg/l), MCPB (µg/l), Mecoprop (µg/l), Diazinon (µg/l), Chlorfenvinphos (µg/l), Propetamphos (µg/l)	flexible	flexible
Microbiological: Coliforms (No./ml), E.Coli (No./ml), Viruses (No./ml), Heterotrophs (No./ml)		
Others: Chlorophyll-a (µg/l), Taste (Number), Odour (Number), Particle Size (µm), Particle Count (No./ml)		Particles