Models for Drinking Water Treatment

Methodology for Integration
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1 Introduction

In Work Package 5.4 “Treatment simulator” of the TECHNEAU project, it is the objective to produce a European platform for modelling of drinking water treatment processes. This document describes the 2nd deliverable of the project, where an approach is proposed to integrate existing models into this platform. In the 1st deliverable a review of the State of the Art of existing models was made. It concluded that OTTER, developed by WRc; Stimela, developed by TU-Delft/DHV and Metrex, developed by Univ. Duiisburg/IWW were the most appropriate existing platforms to act as a base for future development, and integration will focus on these.

During a work package meeting in April 2006, conclusions were drawn about the strong and weak points of the existing models and the requirements for the new modelling platform. The most important conclusion was that the existing models can provide a good starting point for the proposed new platform, and that it is not necessary to re-invent the “modelling wheel”. It was decided to base the new modelling platform upon the existing OTTER system, using the knowledge and strong points embedded in Stimela and Metrex.

The present report gives a summary of the context of the new modelling platform and an approach for producing the prototype that can be demonstrated as the third deliverable 18 months after the start of the TECHNEAU project.
2 Context of new modelling platform

2.1 Strengths and weaknesses of existing modelling platforms
The strengths and weaknesses of OTTER, Stimela and Metrex are summarised below.

Otter
- Models in Fortran
- Easy to build up treatment plant
- Dedicated simulation/integration
- Building on process level and model choice later
- Visualisation and calculations are separated
- Graphically attractive
- Loop detection
- Data in / reports out is easy, using Excel or similar spreadsheets
- Dynamic linking with other programs is possible (COM interface)
- Many models for surface water (excluding biological treatment and softening)
- Proven models (to be improved still)
- Well documented
- Scientific publications (journals, congresses, PhD theses)
- Strictly licensed
- Target group: plant managers/consultancy
- Calibration procedures (spread sheets provided), not automatic
- Difficult to adapt to special requirements (of model)
- Selecting appropriate models for given water quality determinands is not always clear
- Closed source, way of calculation not open (integration method)
- Alive (available but not marketed)

Stimela
- Use of Matlab functionalities (integrator, loop detector, debugging)
- Structural programming of treatment processes based on a predefined format
- Strong, flexible graphical output
- Data in/export is easy
- Scientific publications (journals, congresses, PhD theses)
- Focus on model development
- Linking with other programmes possible
- Still developed
- Large systems require much calculation time
- User interface difficult to use
- Calibration not standardised
• Web interface is limited
• Matlab necessary for calculations (knowing, buying, dependency)
• Documentation is limited
• Target group: model R&D and control

Metrex
• Use of Matlab separated from interface
• Web application possible (Java/HTML)
• Structural programming of treatment processes based on a predefined format
• Integration per process and output can be averaged to next process
• Simulation on different levels
• Fuzzy parameter determination
• Linkage between water quality parameters and processes
• Characterisation of DOC and SS (particles)
• Model building seems laborious
• No loops possible
• Matlab necessary for calculations (fixed integrator: ODE23)
• Target group not known

2.2 Target groups and possible applications for new modelling platform
The new modelling platform is aimed at a broad range of users and for many different applications. These are summarised below:

Target groups
• Consultants
• Operators
• Students
• Researchers
• Regulators

Applications
• Process design
• Troubleshooting
• Incident management (external/internal)
• Operational improvements and optimisation
• Controller design
• Research/ model development
• Testing for robustness of process/ sensitivity analysis
• Compliance with regulations (microbial risk analysis)
• Benchmarking
• Training of operational personnel
• Educational purposes (presentation/design/research)
2.3 **Requirements and availability of new modelling platform**

The new modelling platform should be flexible and easily accessible to members of TECHNEAU and other interested users. Therefore, it was decided to develop a modelling platform that is free of charge with respect to the use of the platform. Other requirements are listed below.

**Requirements**

- Communication with other platforms (e.g. SCADA systems, distribution models)
- Different levels of understanding of processes for different user applications
- Access via web (direct or download or combination)
- Include as many processes as possible to adequately represent the pilot sites.
- Extendable to new determinands and processes
- Easy data handling (import/export)
- Graphical user interface
- Documentation and help facilities (Local language support?)

**Availability**

- Free use
- No open source for users
- Open source for developers
- A mechanism for other users to acquire the source code
- No commercial packages involved at the end user level; commercial packages may be used if they are needed for development, but do not impose run-time or distribution fees to the end users
- Closed platform and closed models

2.4 **Processes and parameters**

The new modelling platform will concentrate on conventional drinking water treatment processes. In the platform some of the processes available in OTTER and Stimela will be incorporated, and extended with the additional processes needed for the evaluation of treatment trains and processes studied in the TECHNEAU project. In Work Package 5.1, coagulation, filtration and conditioning will be examined, and new models potentially developed. In Work Package 5.3 research will also be carried out into bio-filtration. The extension towards new processes such as UV and membrane filtration is still under discussion and depends on the requirements from the other work packages in Work Areas 2 and 5.

The water quality parameters (determinands) that have to be addressed depend on the possible applications. However, emphasis will be given to parameters that are part of European legislation, that influence treatment performance (or other processes) and that influence water quality in distribution networks (e.g. AOC/particles/MAP or corrosion indices.)
2.5 Basis of modelling platform

Based on the evaluations of the existing modelling platforms and the requirements for the new modelling platform, it was decided that the new modelling platform will be based on OTTER. This means that it will have a .net user interface (probably Visual Basic, but possibly C#) and a simulator that is programmed in FORTRAN and C/C++. In addition, the strong points of the other platforms will be incorporated, such as specific models and the web enabling tools of Stimela and Metrex.

The new modelling platform will fulfil the requirements mentioned in this chapter and use of the modelling platform will be free of charge.

WRc will lead the basic programming of the platform, in co-operation with TU-Delft/DHV. The models within the platform will be thoroughly verified and validated. A scientific committee will assure the quality of the models within the platform.
3 Approach for integration of OTTER, Stimela and Metrex

3.1 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 overwhelm 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.

The list of determinands used by OTTER will be extended with the relevant additional determinands used by Stimela and Metrex. Attention will be given to the use of particle size distributions during modelling. Metrex addresses this topic and it is considered important for disinfection modelling and modelling of water quality in distribution networks. However, it requires extra data and modelling and therefore a strategy must be found to include this item in the new modelling platform.

The determinands specified in European legislation will be included in the list of determinands.

TU-Delft will take the lead in determining a first list of determinands.

3.2 Treatment processes

As mentioned before the treatment processes that will be incorporated in the modelling platform are on one hand determined by existing models in OTTER, Stimela and Metrex and on the other hand based on the needs and developments in other work packages in the TECHNEAU project.

TU-Delft will take the lead to providing technical descriptions of the treatment processes in OTTER, Stimela and Metrex to be incorporated in the new modelling platform. WRc will then provide support to integrate the models.

Additional research will be done to extend the number of treatment processes in the platform and to use the platform adequately for operational improvements. Therefore, TU-Delft will recruit a PhD-student to specialise on these topics. Which of the processes must have priority will be discussed with project leaders of parallel work packages.
3.3 Programming, communication and web-access

While water treatment works modelling appears to be a specific research area, it can be regarded simply as 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.

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

- **Modular sequential**: Each module has its differential equations integrated over the period $T_{\text{start}}$ to $T_{\text{end}}$. Each downstream process is provided the outlet streams defined at $T_{\text{start}}$ and $T_{\text{end}}$, and assume a linear variation in flows and water quality between the period $T_{\text{start}}$ and $T_{\text{end}}$.

- **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, with 1000 equations. For explicit integration methods there is little difference between the two, 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 timestep, 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 flagging this up and recalculating all process models. 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.

Events fall into two main categories – those handled as differential equations, and those handled as algebraic equations.
A typical differential event is filling a tank, where the differential equation has a sharp change when the tank is full (there is no further increase in volume, and any additional inflow must appear as an overflow.) 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 upon 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.

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.

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 the 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 – but this means that the timestep is always small, to catch the discontinuity, so that the simulation is inefficient and compute-intensive. Differential solvers usually do not include the handling of algebraic discontinuities, and therefore there is a need to have access to the integrator source code and modify the code slightly. In the new modelling platform this should be revised and different time constants for the different process should be considered.

OTTER differentiates between water quality and water flow rate (water demand), unlike Stimela and Metrex. For both solutions advantages and disadvantages can be given. A final solution for the new modelling platform should be found.

OTTER has a COM interface that was originally designed to permit integration with a SCADA system. The COM interface supports the following actions:

<table>
<thead>
<tr>
<th>Routine</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setup</td>
<td>Open the database containing the simulation files</td>
</tr>
<tr>
<td>CreateNewRun</td>
<td>Create a new run, based on a pre-existing run</td>
</tr>
<tr>
<td>SetValue</td>
<td>Adjust any run parameters. This is usually done at the start of a run, but could be done during a run.</td>
</tr>
<tr>
<td>RunSimulation</td>
<td>Carry out the simulation.</td>
</tr>
<tr>
<td>GetValue</td>
<td>Retrieve calculated values for use by the controlling program</td>
</tr>
<tr>
<td>SaveSimulation</td>
<td>Save the results.</td>
</tr>
</tbody>
</table>
This provides a minimal set of communicating routines, but requires some knowledge of the structure of the simulation to ensure that the use of SetValue and GetValue retrieves the correct data item from the correct location.

The .NET family of languages have been designed with web-enabling as an integral part of the language specification. Therefore, it is possible to make the new modelling platform, based on OTTER, be available through the Internet. Experiences with the web-based modelling by Stimela and Metrex will be used to define the web enabling.

During a session in Autumn 2006, a discussion between TU-Delft and WRc will result in final choices on the above programming options.

3.4 Prototyping
Based on the decisions taken described in the preceding paragraphs a prototype of the software will be developed. WRc will take the lead in this respect and technical descriptions of the software will be defined and circulated.

The prototype will be demonstrated during a TECHNEAU conference in June 2007 and be made available for Work Package 5.4 members for testing.

3.5 Quality assurance
In order to assure the quality of the process models within the new modelling platform a task force will be formed within IWA. This task force will stimulate scientific publications with respect to the individual models, consisting of model description, calibration and validation.

The task force will be formed by members of Work Package 5.4, other specific TECHNEAU members and invited non-TECHNEAU members.

Proposed composition of the task-force:
Luuk Rietveld (TU-Delft, task-force leader)
Glenn Dillon (WRc)
Bjornar Eikebrokk (Sintef)
Junas Talin (Riga)
Achim Maelzer (IWW)

The task force will organise bi-annual workshops of which the first was held in June 2006.

3.6 Planning
1. TU-Delft will prepare a list of required determinands for the new platform, looking at the requirements of EU legislation, common water industry practice in the TECHNEAU countries, and the technical requirements of the proposed process models;
2. TU-Delft will prepare a list of required treatment processes from those available in OTTER, Stimela and METREX;

3. Riga will prepare a list of required treatment processes for the water works involved in the TECHNEAU pilot trials;

4. WRc will prepare the software framework;

5. TU-Delft, WRc and IWW will collaborate in migrating the chosen models from Stimela, OTTER and METREX into the new platform;

6. Sintef, TU-Delft and IWW will collaborate in implementing the new process models developed by the other Work Areas into the new platform;

7. End-September 2006 an internal report will be circulated to WP 5.4 partners and IWW describing the determinands and the algorithmic description of the process models to be migrated from OTTER, Stimela and METREX;

8. End-December 2006 an internal report will be circulated to WP 5.4 members and IWW describing the program structure for the framework;

9. Additional internal reports will be circulated to WP 5.4 partners describing the new models, at the algorithmic level, being proposed in the other Work Areas