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TAPWAT: Definition, structure and applications for modelling drinking-water treatment.

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Abstract

The '**T**ool for the **A**nalysis of the **P**roduction of drinking **WAT**er' (TAPWAT) model has been developed for describing drinking-water quality in integral studies in the context of the Environmental Policy Assessment Function of the RIVM. The model consists of modules that represent individual steps in a treatment process, so that different treatment processes can be constructed. The treatment steps included in TAPWAT are used mainly in systems for the treatment of surface water. The current version of TAPWAT described in this report consists of modules based on removal percentages and on process or semi-empirical modelling. Stochastic modelling using beta-distribution has been worked out for two treatment steps and seems to be a promising technique; however, the availability of data for individual treatment steps is a disadvantage.

In general, this combination works out fairly well in the model structure developed for TAPWAT.
The model must be able to cover, at least for pathogens, the pathway from water source to infection risk for the public. The parts of the puzzle are present, but the puzzle still has to be laid.

The model is as yet only suitable for operation by experts. A plan of action is recommended in which the existing and missing modules, compounds and micro-organisms of interest will be prioritised and the necessary validation of the model described. This plan of action should be implemented to improve the current TAPWAT version and make it suitable for assess public health risks.

Preface

This report describes the main features of the model, TAPWAT, constructed at the RIVM in cooperation with the Delft University of Technology. The project was set up mainly to construct a mathematical model that, could calculate, the removal of micro-organisms and chemicals, on the one hand and the formation of by-products, on the other, on a global spatial scale during the drinking-water production process.
The current version of the model described in this report aims at the treatment of surface water and, in particular, the removal of micro-organisms and the formation of disinfection by-products.

Our thank goes out to the drinking-water supply companies for providing the data used in this project. We also thank our colleagues in Bilthoven and Delft for their useful comments and support during the course of the project.

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Summary

The model, TAPWAT (**T**ool for the **A**nalysis of the **P**roduction of drinking **WAT**er), has been developed for describing drinking-water quality in integral studies in the context of the Environmental Policy Assessment Function of the RIVM. TAPWAT consists of modules that represent individual steps in a treatment process, so that different treatment processes can be constructed. The steps included in TAPWAT are used mainly in systems for the treatment of surface water. The current version of TAPWAT, described in this report, consists of modules based on removal percentages and on process or semi-empirical modelling. In general, this combination works out fairly well in the model structure developed for TAPWAT.

Modules based on removal percentages
Removal percentages and ranges are derived from existing database, found in the literature and derived from pilot and full-scale treatment plants. There is a lack of measurement data, especially for the individual treatment steps and target compounds like pathogenic micro-organisms and pesticides. About 15% of the ranges are based on detailed data from water-supply companies.
Of the data on five micro-organisms of interest for public health or an indicator, only data for spores of sulphite-reducing clostridia (SSRC) are available. The removal of pathogenic micro-organisms is based on numbers of logarithmic reduction derived from field studies or experiments at pilot treatment plants.

For the organic micro-pollutants and heavy metals (six compounds), data availability is very limited and even absent for two compounds. Data availability is reasonable for disinfection by-products. Validation is done for two parameters in an example of a treatment process, it worked out well for the data-rich parameter. The uncertainty of the percentage ranges is the lowest when the ranges are derived from full-scale treatment plants.

Modules based on process or semi-empirical modelling
In TAPWAT the chlorination and ozonation modules are incorporated for the prediction of disinfection by-products and the removal of micro-organisms. These modules are based on empirically based equations. Examples for the prediction of the formation of disinfection by-products give reasonable results. Stochastic modelling is done for two treatment steps (floc formation and removal, and activated carbon filtration). Stochastic modelling using beta-distribution is a promising technique; however, the lack of available data from individual treatment steps is a disadvantage. Only indicator parameters or parameters which are easy and cheap to measure are suitable.

Model calibration and validation
Data from full-scale treatment plants should be used as much as possible for model calibration and validation, both for percentages and the process modules of TAPWAT. The availability of data is limited, especially for individual treatment steps and non-system parameters like pesticides. Pilot-scale and laboratory data will have to fill the (many) gaps.

Only a few validations are done with TAPWAT. For the most interesting parameters like pesticides and pathogens, either data is lacking or there are too many measurements below detection limit. Indicators should be used for the pathogens; however, there are still a lot of

'below-detection-limit' data. The subject on how to calculate the removal of micro-organisms has been described in a separate report (Evers and Groennou, 1999).

General expressions for the estimation of value μ (average in the beta-distribution) should be formulated for use in stochastic modelling. This value is specific for each treatment plant but can be made more general to improve of the usefulness of TAPWAT, for example, by analysing measurement data of more plants in the same way.

The modules in TAPWAT are based on an average performance of treatment steps; this can differ from the performance of a treatment step in a particular treatment system.
Caution will be needed when applying the model to specific cases. The main goal of TAPWAT is to use the model in global-scale studies for the Netherlands.

Recommendations
TAPWAT is a model suitable for application on a global scale in treatment plants using, surface water as the raw water source. The model described is not yet completed. The modules based on removal percentages should be updated regularly, and those based on process or semi-empirical modelling have to be validated for more systems, so that the uncertainty of the results can be described on a higher level.

New model studies for soil passage have been recently published (Schijven, 2001), the results of which should be incorporated in TAPWAT. Considering that the UV-disinfection technique has now become more important for the removal of pathogens like viruses and protozoa, a module for UV should be incorporated in TAPWAT. Membrane technology is used more and more for piped water production like drinking water and household water. Information available from pilot and full-scale plants should be used to improve the existing modules.

The model must be able, at least for pathogens, to cover the pathway from water source to infection risk for the public. The parts of the puzzle are present but the puzzle still has to be laid.

The model is as yet only operable for experts. To make it suitable for non-experts an update of the current version with input screens etc. has to be made. This work should be put out to a contractor.

A plan of action is recommended in which the existing and missing modules, compounds and micro-organisms of interest are prioritised and the necessary validation of the model carried out. To both improve the current TAPWAT version and make it also suitable for public health risk assessment the plan of action should be carried out by experts and model updates eventually put out to a contractor.

Samenvatting

Het model TAPWAT (**T**ool for the **A**nalysis of the **P**roduction of drinking **WAT**er), is ontwikkeld om de drinkwaterkwaliteit te beschrijven voor integrale studies in het kader van de planbureaufunctie van het RIVM. Het model bestaat uit modules die de individuele zuiveringsstappen van het drinkwaterzuiveringsproces vertegenwoordigen. De zuiveringsstappen in TAPWAT worden voornamelijk gebruikt in systemen voor de behandeling van oppervlaktewater. De huidige versie van TAPWAT, zoals in dit rapport beschreven, bestaat uit modules gebaseerd op verwijderingspercentages en modules gebaseerd op proces of semi-empirische modelering.

Modules gebaseerd op verwijderingspercentages
Verwijderingspercentages and ranges daarvan zijn verkregen vanuit bestaande databestanden, uit de literatuur, vanuit proefinstallaties en van volledig in bedrijf zijnde zuiveringsstations. Er is een gebrek aan meetgegevens vooral voor wat betreft de individuele zuiveringsstappen en voor de belangrijke parameters zoals pathogene micro-organismen en bestrijdingsmiddelen. Ongeveer 15% van de ranges zijn gebaseerd op gedetailleerde gegevens van waterbedrijven. Van de vijf micro-organismen van belang voor de volksgezondheid of als indicator-organisme hiervoor, zijn er uitsluitend gegevens voor sporen van sulfiet reducerende clostridia beschikbaar. De verwijdering van pathogene micro-organismen is gebaseerd op aantallen logaritmische eenheden reductie verkregen uit veldstudies of uit experimenten met proefinstallaties.

De beschikbaarheid van gegevens voor de organische micro-verontreinigingen en zware metalen (zes stoffen) is erg beperkt en de gegevens voor twee stoffen zijn zelfs afwezig. De beschikbaarheid van gegevens is redelijk voor desinfectiebijproducten. Validatie is uitgevoerd voor één casus en twee parameters, en werkt goed voor een parameter waarvoor veel gegevens beschikbaar zijn. De onzekerheid in het percentage ranges is het laagst wanneer de ranges afkomstig zijn van volledig in bedrijf zijnde zuiveringsstations.

Modules gebaseerd op proces of semi-empirische modelering
In TAPWAT zijn de modules chloring en ozonisatie aanwezig om de verwijdering van micro-organismen te beschrijven en de vorming van desinfectiebijproducten te voorspellen. Deze modules zijn gebaseerd op empirisch verkregen formules. Voorbeelden van de voorspelling over de vorming van desinfectiebijproducten geven redelijke resultaten. Stochastische modelering is uitgevoerd voor twee zuiveringsstappen (vlokvorming en vlokverwijdering en voor actieve koolfiltratie). Stochastische modelering met behulp van de beta-verdeling is een veel belovende methodiek hoewel de geringe beschikbaarheid van data voor de individuele zuiveringsstappen een nadeel is.

Model calibratie en validatie
Gegevens afkomstig van zuiveringsstations zullen zoveel mogelijk gebruikt dienen te worden voor modelcalibratie en modelvalidatie, zowel voor percentage als voor procesmodules in TAPWAT. De beschikbaarheid van gegevens is beperkt vooral voor individuele zuiveringsstappen en niet-systeemparameters zoals bestrijdingsmiddelen. Proefinstallaties en laboratoriumgegevens zullen de vele gaten in het databestand moeten vullen.

Er is een beperkt aantal validaties uitgevoerd met het model TAPWAT. Voor de meest interessante parameters als bestrijdingsmiddelen en pathogenen is er een tekort aan gegevens

of zijn er teveel metingen beneden het detectieniveau. Voor de pathogenen zullen indicatoren gebruikt moeten worden maar ook dan zijn er veel meetresultaten beneden de detectiegrens. Het onderwerp hoe de verwijdering van micro-organismen te berekenen is beschreven in een separaat rapport (Evers en Groennou, 1999).

Als stochastische modelering gebruikt wordt zullen algemene uitdrukkingen voor de schatting van de waarde μ (gemiddelde in de beta-verdeling) dienen te worden vastgesteld. Deze waarde is specifiek voor elk zuiveringsstation maar kan meer algemeen worden gemaakt in het belang van de bruikbaarheid van TAPWAT. Een mogelijkheid om dit uit te voeren is om meetgegevens van andere stations op dezelfde manier te analyseren.

De modules in TAPWAT zijn gebaseerd op de gemiddelde prestatie van zuiveringsstappen; dit kan afwijken van de prestatie van een zuiveringsstap in een individueel zuiveringsproces. Voorzichtigheid is geboden met het gebruik van het model voor specifieke systemen. Het belangrijkste doel van TAPWAT is om het model te gebruiken voor globale studies binnen Nederland, zogenaamd landsdekkend.

Aanbevelingen
TAPWAT is een model dat gebruikt kan worden op globale schaal voor zuiveringsstations die oppervlaktewater als bron gebruiken. Het in dit rapport beschreven model is nog niet compleet. De modules gebaseerd op verwijderingsspercentages zullen regelmatig geüpdate moeten worden, de modules gebaseerd op proces of semi-empirische modelering dienen voor meer systemen gevalideerd te worden zodat de onzekerheid in de resultaten beter beschreven kan worden.

Recent zijn nieuwe studies gepubliceerd (Schijven, 2001) voor bodempassage, deze zullen in TAPWAT geïncorporeerd worden. De techniek UV-desinfectie wordt steeds belangrijker voor de verwijdering van pathogenen als virussen en protozoa. Een module hiervoor zal in TAPWAT geïncorporeerd dienen te worden. Membraantechnologie wordt meer en meer gebruikt voor de productie van leidingwater als drink- en/of huishoudwater. Beschikbare informatie van proefprojecten of in bedrijf zijnde zuiveringsprocessen kunnen gebruikt worden om de bestaande modules te verbeteren.

Het model moet in staat zijn om het gehele pad te beschrijven van bron tot en met infectierisico voor de bevolking (tenminste voor pathogenen). De delen van de puzzel zijn beschikbar maar de puzzel dient nog wel in elkaar gezet te worden.

Het model is nu alleen geschikt voor ‘experts’. Om het voor een breder publiek geschikt te maken zal de huidige versie uitgebreid moeten worden met bijvoorbeeld invoerschermen. Aanbevolen wordt dit onderdeel uit te besteden.

Aanbevolen wordt een plan van aanpak te maken waarin de bestaande en de nog missende modules, stoffen en micro-organismen worden aangegeven. De implementatie hiervan in TAPWAT dient vervolgens geprioriteerd te worden in de tijd evenals de noodzakelijke validatie van het model. De verbetering van de huidige versie van TAPWAT en de voorgestelde slag om het model geschikt te maken voor risicoanalyse ten behoeve van de volksgezondheid zal volgens het plan van aanpak uitgevoerd moeten worden door deskundigen of desnoods worden uitbesteed.

1 Introduction

The main goal of the department of environmental research of the National Institute of Public Health and the Environment (RIVM) is to produce general reports for the Dutch government. The main products are:

- State of the environment 'Milieubalans'
- State of the nature 'Natuurbalans'
- Environmental outlook 'Milieuverkenningen'
- Nature outlook 'Natuurverkenningen'

In these reports subjects are presented for which the activities of the society have a negative effect (pressure) on nature and environment. Some examples of these subjects are the consumption of energy, the production of carbondioxide by the traffic, which are reported at one side. At the other side the quality of water, soil and air is reported in relation with environmental themes as acidification, eutrophication and climate change. In the 'State of the environment' the purposes of the government to improve the quality of the environment are confronted with the state of the quality of the environment. For this purpose, indicators are used focussing on the subject drinking water e.g. the quality of the sources for drinking water related to nitrate and pesticides. The quality of the product drinking water is classified as an effect on public health.

To be able to produce these reports the whole chain of drinking-water production from source to tap is reviewed. For this purpose mathematical models are constructed for various subjects. In this report one of these models named TAPWAT is presented. TAPWAT means **T**ool for the **A**nalysis of the **P**roduction of drinking **WAT**er. TAPWAT is a tool to predict the purification efficiency of a drinking-water production plant used to purify surface water and/or ground water into drinking water. The input for TAPWAT is the raw water quality for chemicals and micro-organisms. The output is the quality of the drinking water for the parameters, which can be analyzed by the model. For this, the complete purification process was split up in physically separate units. The model can be simple: a module with only a removal percentage for certain parameters or a description of the water treatment process in model formulations in a process module. In chapter 2 the principles of the model are described; in chapter 3 the concept is described and the chapters 4 and 5 the technical modules (percentages and process) are described. Chapter 6 give the main results of the stochastic modelling, chapter 7 gives examples of validation, applications of the model and chapter 8 gives conclusions and recommendations. In a separate report the modules are described in more detail (Rietveld et al., 2001).

2 Definition of the model TAPWAT

In this chapter information is presented about the realisation of the model TAPWAT except the technical information. This information is based on the definition study of TAPWAT (Kragt et al., 1996).

2.1 Goals of the model

The main applications of the model are:

- 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.

The model is developed according two pathways: empirical or percentages and process modules. The modules are incorperated in one modelstructure so the modules from both pathways can be used for one application. The model is developed according RIVM standards for information infrastructure and modelling.

2.2 Parameters and treatment steps

In the definition study all available treatment steps at one side and all for drinking water relevant micro-organisms and chemical compounds at the other side were studied. This resulted in a long list with parameters and treatment steps.
Review of this list and expert judgement resulted in a matrix with parameters and treatment steps which had the priority to be modelled (Kragt et al., 1996).

The following parameters were chosen for different reasons as a representive of the group or the availability of data or expected to be a relevant problem:
Micro-organisms: *Giardia*, *Cryptosporidium*, enteroviruses and their indicators
Pesticides: atrazin, glyfosaat and 1,2-dichloropropane
Disinfection byproducts: bromate and trihalomethanes
Metals: nickel, cadmium, chromium
Process parameters: pH, temperature, DOC, turbidity and bromide.

The following treatment steps were chosen because they are a part of surface water treatment and they have the capacity to remove the interesting compounds:
Storage reservoir, chlorination, ozonation, floc formation/floc removal, rapid sand filtration, activated carbon filtration, membrane filtration and slow sand filtration.

2.3 Approach of modelling

2.3.1 Percentage removal

Information was collected from literature, reports, data from production plants and sometimes expert judgement to design ranges of percentages for removal micro-organisms and compounds by the selected treatment steps. This process is described in chapter 4.
Data from production plants were prefered above pilot plant data or laboratorium experiments. But data of production plants for the chosen compounds and individual treatment steps are scarce.

For compounds like metals and pesticides modules based on removal percentages will be good enough for the purpose for which TAPWAT is used. This all results in a number of modules based on ranges of removal percentages which can be used for global sudies. Monte Carlo analysis can be used to find the most probable result when more parameters are used for calculations.

2.3.2 Process or semi-empirical modelling

The design of a process module was done following a sjabloon, a test procedure plan including reporting of the results. In chapter 5 of this report a short description is given for a few modules especially chlorination and ozonation which are used in the current version of the model TAPWAT. More details can be find in internal documents and in Rietveld et al., 2001.

2.3.3 Stochastic modelling

The beta-distribution is used for statistical analyses of data of production plants especially for the removal of TOC and turbidity by flocculation and floc removal and activated carbon filtration. This statistic technique is useful to develope empirical models if enough data of individual parameters from production plants are available.

2.4 Applications of TAPWAT

The model will be used to describe the drinking-water quality in integral studies, examples are given in the last chapter of this report. The connections with other models are still under construction in a separate project.

3 The concept of the model TAPWAT

3.1 Introduction

In this chapter the principles forming the basis for the realisation of the model TAPWAT will be described. These principles will be based on the definition study of TAPWAT (Kragt et al., 1996), an outline of which is included in the previous chapter. A complete description of the technical concept of TAPWAT can be found in the LWD-report 'Ontwerp modelstructuur van TAPWAT' (van Gaalen et al., 1999). A number of aspects mentioned in the definition study (Kragt et al., 1996) serve as starting points for the technical concept of TAPWAT. These aspects will be summarised below.

3.2 Basic principles from the definition study

For the purpose of flexibility the model will consist of modules that represent individual treatment steps in a treatment system. This concept offers the possibility to build different treatment systems by means of a library of modules, as well as allowing replacement of modules by improved ones.

The necessary in- and output can differ for every combination of module and substance. To allow for flexible applicability and interchangeability of modules, it is necessary for them to communicate by means of a general interface, with which all the required information can be exchanged. Communication doesn't take place directly between modules, but by way of a general part of the model that henceforth will be called the *model structure*. In a central database, that constitutes part of the model structure, the information to be exchanges will be stored (temporarily).

The model structure will also have to provide for the possibility of putting together a treatment system on the basis of available treatment modules and for the communication between the model and the user. This concept is schematically shown in Figure 3.1.

The model will be built in the MATLAB/Simulink-environment on MS-Windows-PC's.

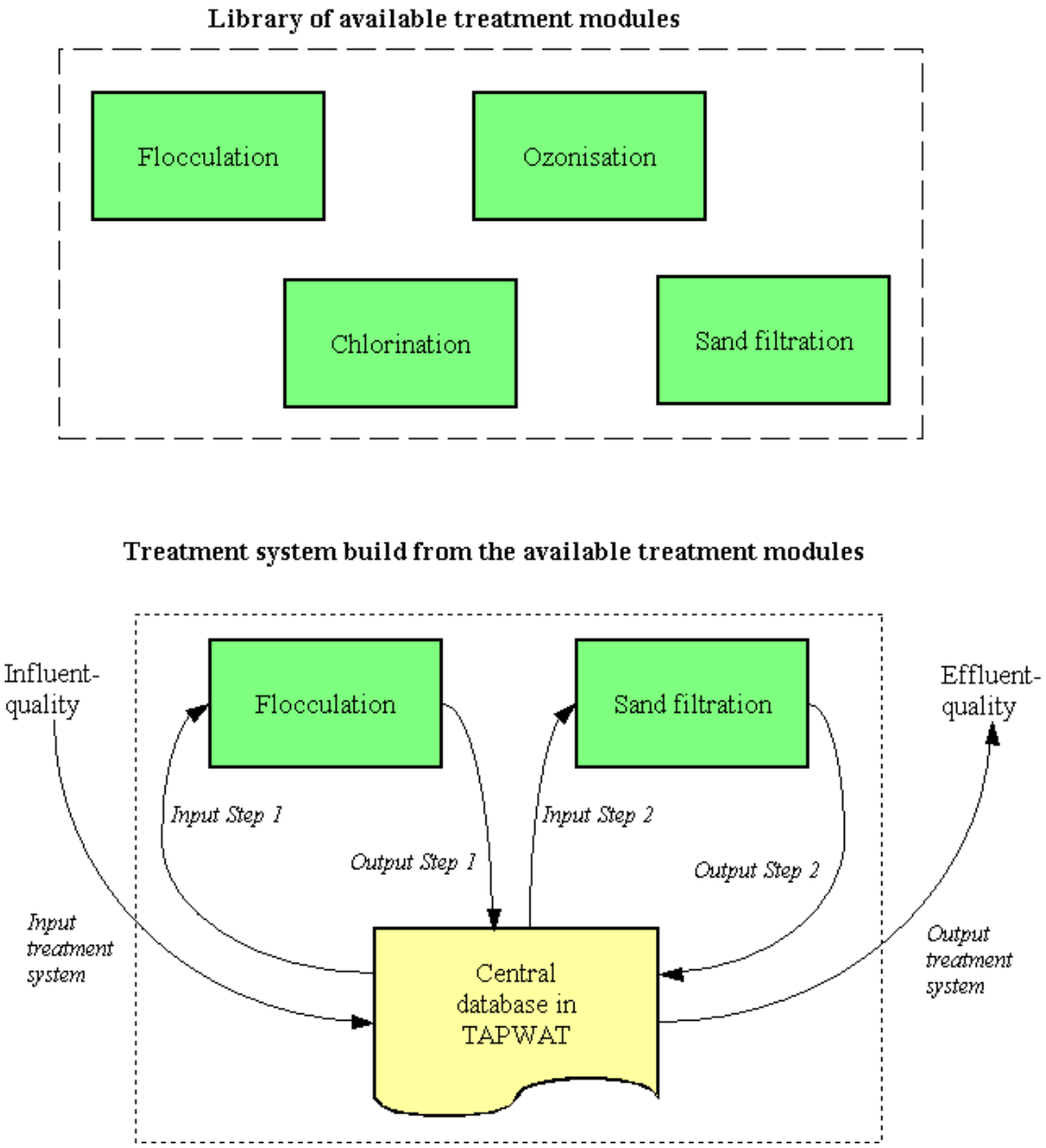

Figure 3.1 Concept of the model structure of TAPWAT

3.3 Input and output of TAPWAT

In this paragraph the required in- and output of the model will be examined, as well as the form in which it can be entered.

3.3.1 Input data

The input of TAPWAT, i.e. the data to be provided by the user in order to perform a calculation, consists of:

- The composition of the treatment system concerned (which treatment modules in what order);
- Design- and process parameters of the treatment steps present in the treatment system (design parameters are considered as fixed after building the step; process parameters can be changed after building the step to influence the performance of the process);
- Starting conditions of the treatment steps present in the treatment system;

- Name and concentration in raw water of the substances or substance groups to be purified (i.e. to be calculated), possibly substance properties also;
- Name and concentration in raw water of other quality parameters that can influence the amount of purification.

Not all information is needed for every module. The person building a module determines what input is required, on the basis of the kind of modelling to be pursued and the complexity of the processes described. The input needed will be stated in the specifications of a module; in this way a user will know what input the model expects.

3.3.2 Specification of the input files

The following ten input files will be used to provide TAPWAT with the necessary information:

- General run data: these determine a number of general aspects of the calculations to be performed, such as the time period to be considered and the number of draws to be performed in the Monte Carlo analysis (see 3.5);
- Composition of the treatment system and the substances to be calculated;
- Design- and process parameters;
- Input concentrations;
- Starting conditions;
- Substance groups;
- Substance properties;
- Relation modules – treatment steps; this relation enables every module to use the values of the design/process parameters relating to the step and the treatment station concerned;
- Removal percentages of simple empirical modules: name module, name substance, removal percentage. For the purpose of the simple empirical modules (consisting of a single removal percentage or range of percentages) only one module will be built, that will read the percentages to be used from this file;
- Model parameters: values of the parameters that will be used in the modules. This concerns the parameters for which a value or range of values is determined during calibration.

The names of modules, treatment steps, design/process parameters, substances, substance groups, substance properties, starting conditions and model parameters must be unique. To ensure this, lists of names must be kept in one location only; every module has to use the names defined in these lists.

3.3.3 Output data

The output of TAPWAT consists of:

- Concentrations in the resulting drinking water of the substances or substance groups to be purified (i.e. to be calculated), during a given time period;
- Concentrations in the resulting drinking water of other quality parameters that can influence the amount of purification, during a given time period;

The properties of the substances can also be part of the output of the model, if these have been changed during the treatment process.

3.3.4 Specification of the output files

The results of the calculations are written to output files, with a new file for every treatment system. For every combination of treatment step, time step and substance more than one output concentration can be calculated: that is, one for every set of drawings for the Monte Carlo analysis (see paragraph 3.5 for a description of Monte Carlo analysis).

Awaiting the standard functions for the HF11-format, the output files will have a structure similar to the input files: ASCII with a fixed layout.

3.4 Input and output of a treatment module

In this paragraph will be specified what information has to be exchanged between treatment modules by way of the general interface: the model structure.

3.4.1 Input of a treatment module

During calculations with TAPWAT the following information serves as input for each of the treatment modules:

- Information concerning the substances or substance groups to be purified: name, concentration in the incoming water (influent) and possibly substance properties;
- Information concerning the other quality parameters that can influence the amount of purification: name, concentration in the incoming water;
- Information concerning the treatment step: values of the design- and process parameters of the treatment step.

3.4.2 Output of a treatment module

The output of a treatment module is mostly identical to the input; this output will often serve as input for the next one. So the output of a module consists of:

- Information concerning the substances or substance groups to be purified: name, concentration in the outgoing water (efluent) and possibly substance properties;
- Information concerning the other quality parameters that can influence the amount of purification: name, concentration in the efluent.

The output of a module can differ from the input in:

- The concentration of the substances;
- The properties of the substances; it is not clear yet if this will be used in the model.

3.5 Monte Carlo analysis in TAPWAT

To be able to determine the uncertainty of the results, Monte Carlo analysis will be used in TAPWAT. This has the following consequences:

- As input for the model multiple values will be used instead of single. As far as known the uncertainty of every input item will be stated in the form of a range of values and if necessary a distribution of the values within the range.
- For every time step the calculation will be performed not once, but the number of times as stated by the user in the input file with general run data (see 3.3.2). For every calculation a new aselect draw will be performed from each of the given input ranges. With these drawn values the calculation will be performed once, after which new draws are made for the next calculation, etc.

- The result will be not one outcome per time step, but as many as stated by the user in the input file with general run data. On these results statistical processing can be performed, such as determining percentiles, minimum/maximum and median.

So, for every time step a range of results is available instead of a single value. This range represents the cumulative effect of the given uncertainties of the input items.

3.6 Steps to be performed by the model

To perform calculations the following steps have to be passed through within the model:

- The information concerning the composition of the treatment system is read from the input file and processed: i.e. the treatment modules are linked in the right order to form the complete treatment system.
- The information concerning the quality of raw water (substances, substance groups, substance properties and concentrations) and concerning the treatment steps to be used (design/process parameters, starting conditions, model parameters) is read from the input files and stored in the central database of the model.
- On behalf of the Monte Carlo analysis, draws are performed from the given ranges of values for each of the input items.
- With every complete set of drawn values (consisting of one drawn value for every input item), the treatment system as built in step 1 is calculated. All the information needed by a module is provided for by the model structure.
- The drawn values for the concentrations of the substances in raw water are offered to the first module; every following module is given the output concentrations calculated by the previous module.
- For every set of drawn values, the results of the calculation (i.e. the concentrations present in the central database of the model after having gone through all the treatment modules) are stored. After having performed the number of calculations stated by the user in the input file, all these results are written to an output file.

4 Determination of removal percentages

4.1 Introduction

In this chapter the so called percentages approach of the model is described. For each treatment step or combination of steps, data present in databases at RIVM, water companies and in the literature were collected to calculate removal percentages for micro-organisms and substances. This work resulted in percentage modules for treatment steps or combination of treatment steps based on ranges presented at the end of this chapter. The ranges make it possibel to use Monte Carlo simulation. A statistical appoach of the data of the production plants resulted in the use of a beta-distribution.

4.2 Removal percentages based on data from databases and literature

On the basis of information available at RIVM and in literature, single percentages and percentage ranges have been determined for the removal of substances and micro-organisms. The following information has been taken into account:

- The so-called REWAB-module in ISDIV (the information system for drinking water and industrial water at the RIVM). This module contains information, delivered by the Dutch drinking-water companies, concerning the quality of water before, during and after drinking-water production. Unlike the company data mentioned above, this concerns figures aggregated over a year.
- Literature relating to drinking-water treatment in the Netherlands.
- Literature relating to drinking-water treatment outside the Netherlands.

The aim was to find the minimum and maximum removal percentage for every combination of treatment step and substance. Based on expert judgement, improbable extremes have been skipped. In case of a choice of figures from several sources, priority has been given to company data over literature; literature concerning Dutch production plants has been given priority over literature concerning foreign plants.

The results of this inventory are incorporated in the concluding table as shown in 4.2.

4.3 Removal percentages based on data of drinking-water production plants

The main part of the data that were used initially in the TAPWAT-project comprise of foreign, laboratory and pilot-scale data. Only a minor part of the data was based on full scale data of Dutch drinking-water production plants, whereas this type of data was considered to be the most important. For this reason, and also in order to obtain process, design and water quality parameters for modelling, additional data were obtained from a number of Dutch drinking-water production plants.

Table 4.1 gives the list of compounds and micro-organisms that was investigated.

Table 4.1 List of investigated compounds and micro-organisms.

Compounds	Disinfection byproducts	Micro-organisms
atrazin	Trichloroacetic acid	*Giardia*
glyphosate	Trichloromethane	*Cryptosporidium*
bentazon	Bromate	Enteroviruses
MCPP	Bromodichloromethane	SSRC
diuron		
nickel		

Three calibration methods were applied. The first method is linear regression. The available measurement pairs are analyzed with the model Y = aX, with X and Y measurement values, and in the purification process the sampling point for X preceeds the sampling point for Y. The resulting point estimate for the parameter *a* has to be transformed to a removal percentage *p* by the formula *p* = 100 x (1 - *a*). The 95% confidence limits, that also have to be transformed by the same formula, will be taken as minimum and maximum borders for a removal percentage range, that can be used for Monte Carlo simulations, for instance. Values lower than 0% and higher than 100% will have to be corrected to 0% and 100%, respectively, to obtain realistic values that can be used e.g. for calculations of a complete purification process.

The second method uses a (cumulative) distribution of removal percentages. First, the removal percentage p of each (X,Y)-pair is calculated (see also above). The removal percentage is set at -1E99 for measurement pairs where the inflow measurement equals zero. From the resulting set of removal percentages, the median or 50% percentile value is taken as a point estimate. For the minimum and maximum borders for a removal percentage range, the 2.5% and 97.5% percentile values are taken.

The third method is applied when only one measurement pair is available. It comprises simply of calculation of the removal percentage for this measurement pair.

Pathogenic micro-organisms
For pathogenic micro-organisms the calculations were done with three data sets:
- The original data set;
- A set in which the inflow measurements that equal zero are set to 1;
- A set in which the outflow measurements that equal zero are set to 1.

Organic micropollutants and heavy metals
If one or more measurements are below the detection limit, the calculations are performed with two data sets:
- A set in which the inflow and outflow measurements that are below the detection limit are set to zero and the detection limit, respectively;
- A set in which the inflow and outflow measurements that are below the detection limit are set to the detection limit and zero, respectively.

Disinfection by-products
For the chlorination step, a specific linear regression model has to be applied, since in this case there is no percentage removal, but formation of compounds. The general model applied is Y = a + X, where X and Y are the concentrations before and after chlorination,

respectively. The parameter a represents the increase in disinfection byproduct concentration due to chlorination. For bromodichloromethane, the model is Y = a, since there is no information available on X.

Also for the chlorination step, the cumulative distribution method is performed in analogy with the general description above, but using the set of concentration increases instead of removal percentages. In general, if one or more measurements are below the detection limit, the analysis is performed as described for organic micropollutants and nickel.

Ranges
The results of the present study are now used to obtain a table with ranges that can be used in a Monte Carlo analysis. For the lower and upper border of the range, the 2.5 and 97.5% percentile values are used or if necessary the values of the one pair method. For pathogenic micro-organisms, the point estimates of the percentiles are used, and for compounds the average is taken of the range for a percentile value. If values for two flows are available, then the average of these values is taken. Negative values are set to zero.

4.4 Determination of removal percentages based on results of treatment plants

The removal of compounds and micro-organisms and the formation of disinfection by-products is summarized for different treatment steps of the following treatment plants:
- WRK III-Water production location Prinses Juliana
- WRK I/II-Water production location ir. Cornelis Biemond
- WNWB-Zevenbergen
- WBE-Kralingen
- PWN-Andijk

The complete set of results of the treatment plants are presented elswhere. The ranges are determined by the 2.5 and the 97.5 percentiles, for the lower and upper border of the range.

The following basic principles have been applied in establishing the table:
- Priority has been given to the ranges based on detailed company data (as described in 4.3), provided that the number of measurements used was sufficiently large to enable reasonably reliable results.
- For turbidity and micro-organisms ranges have been compiled on the basis of detailed company data using the minimum and maximum removal as encountered in the individual treatment systems examined. In this way justice is done to the importance of peak amounts of micro-organisms for determining health effects.
- For all other substances, ranges have been determined on the basis of detailed company data by taking the average median of the individual treatment systems and the average distance between the minimum and maximum removal with regard to the median. This method is based on the idea that for most substances the long term health effects are what matter and not incidental peaks.
- Where no information based on detailed company data was available, use has been made of the ranges determined as described in 4.2.

The results used for the percentage modules of TAPWAT are presented in tabel 4.2 in the bold font. Ranges in regular font are based on literature and RIVM/TUD-data (i.e. the activities described in 4.2); ranges in bold font are based on detailed company data (i.e. the activities described in 4.3). Blanks indicate combinations of treatment step and substance/micro-organism for which no range could be determined.

4.5 General conclusions from the data analysis

Data availability

- Due to the limited number of sampling points, not all purification steps can be analysed seperately. Coagulation/flocculation/sludge blanket separation + rapid filters is the most important example.
- Of the five micro-organisms of interest, only data for spores of sulphite-reducing clostridia (SSRC) are available.
- For the "organic micro-pollutants and heavy metals (six compounds) data availability is very limited and absent for two compounds.
- Data availability is reasonable for disinfection by-products.

Statistical analysis

The non-normal nature of microbial counts and the high number of zero measurements makes linear regression and the percentile method, respectively, less useful. Application of an alternative statistical analysis, using e.g. the betabinomial approach (Teunis et al., 1997), could be useful.

For organic micropollutants and heavy metals, a picture of broad ranges or zero emerges. This is caused by the very limited number of data pairs (1-2) in combination with measurements below the detection limit.

The data for disinfection by-products are characterized by a reasonable number of measurement pairs and a limited number of measurements below the detection limit. This results in realistic estimates for the ranges of removal percentages and produced concentrations in the purification steps.

Point estimates and ranges

Useful point estimates and ranges of removal percentages (and produced concentrations) are only available for disinfection by-products. For organic micropollutants and nickel determination of point estimates and ranges is hampered by data availability and measurements below the detection limit. For SSRC, zero measurements is the main problem.

Comparison with data from literature

- The amount of overlap in the data of the present study and those collected from literature.
- The present study gives generally equal or lower values for removal percentages for corresponding cases, leading to a lowering of the percentages used for TAPWAT calculations for these cases.
- The comparison indicates that literature data (main part of previously collected data) might overestimate in general the removal that is realised in full scale drinking-water production plants.

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Usefulness of full scale data for model calibration
The usefulness of full scale data for model calibration is limited, due to limited data availability. These data are important, however, and should be used as much as possible for model calibration. Pilot-scale and laboratory data will have to fill in the (many) blanks.

Table 4.2 Removal percentages of compounds and micro-organisms and the formation of disinfection by-products expressed as ranges as used in TAPWAT 1.0.

	Reservoir	*Conditioning*	*Chlorination*	*Safety chlorination ClO2*	*Microsieves*	*Coagulation/ flocculation/ rapid filtration*	*Flocculation/ filtration**
Atrazin	0-20	0-0	0-12.5	0-0	0-0	0-20	0-20
Diuron	0-25	0-0	0-0	0-0	0-0	20-20	20-20
Cadmium	60-80	0-0	0-0	0-0	0-0	20-82	20-82
Chromium	75-80	0-0	0-0	0-0	0-0	60-93	60-93
Nickel	0-0	0-0	0-0	0-0	0-0	**-3.7-2.5**	20-60
Enteroviruses	99-99.9999	0-0	99-99.99	90-99.9	0-0	90-99	90-99
Cryptosporidium	68.4-99	0-0	0.76-5.8	0-0	0-0	99-99.7	68.4-99.7
Giardia	68.4-99	0-0	27-99	0-90	0-0	99-99.7	68.4-99.9
Bromate	0-0	0-0	0-0	0-0	0-0	0-0	0-0
Trichloromethane	40-85	0-0			0-0	0-0	0-0
Bromodichloro-methane	35-80	0-0			0-0	0-0	0-0
Simazin	0-0	0-0	0-0	0-0	0-0	0-20	0-20
Dimethoate	0-0	0-0	0-0	0-0	0-0	20-60	20-60
MCPA	0-0	0-0	0-0	0-0	0-0	60-60	60-60
MCPP	0-0	0-0	0-0	0-0	0-0	60-60	60-60
DOC	7.7-9.8	0-0	0-0	0-0	0-0	**10.6-45.3**	10-45
Tubidity						**64-99.6**	
Trichloroacetic acid							
SSRC	**0-100**					**96-99.9**	

*If applicable, the combination of treatment steps *Coagulation/flocculation/rapid filtration* should be used instead of the individual steps
bold font: data are based on detailed company data
regular font: data are based on RIVM/TUD data available.

Table 4.2 continued.

	*Flocculation /settling **	*Flocculation/ flotation/ rapid filtration**	*Sludge blanket separation/ rapid filtration**	*Rapid filtration*	*Slow sand filtration*	*Infiltration / extraction*	*Ozonation*
Atrazin				0-0	0-0	45-66	25-35
Diuron					0-0		73-73
Cadmium				0-15	0-0	15-50	0-0
Chromium				0-0	0-0	23-60	0-0
Nickel					0-0	25-60	0-0
Enteroviruses				0-0	97-100	99.9999-100	99-99.9
Cryptosporidium				0-0	94-100	94-100	45-79
Giardia				0-0	94-100	94-100	79-99
Bromate	**0-0**				0-0	0-0	
Trichloromethane					0-0	75-99	0-0
Bromodichloro-methane					0-0	65-98	0-0
Simazin				0-35	0-0	45-68	20-27
Dimethoate					0-0	58-60	50-94
MCPA				0-3	90-99	90-99	50-75
MCPP					90-99	90-99	6.7-91
DOC	**5.4-41.4**	**10.6-45.3**		**9.8-34.5**	0-0	0-0	0-0
Tubidity	**-169-98.2**	**64-99.6**		**46.8-97.4**		0-0	
Trichloroacetic acid							
SSRC	**6-89.7**	**96-99.9**	**98-100**	**88.9-99.4**			

*If applicable, the combination of treatment steps *Coagulation/flocculation/rapid filtration* should be used instead of the individual steps
bold font: data are based on detailed company data
regular font: data are based on RIVM/TUD data available.

Tabel 4.2 continued

	Activated carbon filtration	*Aeration*	*Hyperfiltration*	*Nanofiltration*	*Ultrafiltration*	*Microfiltration*
Atrazin	20-90	0-0	90-99	65-98	0-0	0-0
Diuron	90-99	0-0	60-99	45-90	0-0	0-0
Cadmium	45-60	0-0	75-98	98-99	20-82	20-82
Chromium	40-70	0-0	72-96	96-99	60-93	60-93
Nickel	0-0	0-0	85-85	96-99	20-60	20-60
Enteroviruses	0-0	0-0	99.9-99.9999	99.99-99.99997	99-99.99997	90-99.9
Cryptosporidium	0-0	0-0	99.9-99.9997	99.99-99.9997	99.9-99.9997	99.99-99.999
Giardia	0-0	0-0	99.9-99.9997	99.99-99.9997	99.9-99.9997	99.99-99.999
Bromate	0-3.3	0-0	75-96	0-0	0-0	0-0
Trichloromethane	**-239.4-33.0**	44-80	70-95	70-95	0-0	0-0
Bromodichloro-methane	**0-7.2**	42-90	70-95	70-95	0-0	0-0
Simazin	35-90	0-0	78-95	65-95	0-20	0-20
Dimethoate		0-0			20-60	20-60
MCPA	50-99	0-0	75-99	75-98	60-60	60-60
MCPP	50-99	0-0	73-99	76-98	60-60	60-60
DOC	**16.4-45.8**	0-0	90-99		0-0	0-0
pH						
Tubidity						
Trichloroacetic acid						
SSRC						

bold font: data are based on detailed company data
regular font: data are based on RIVM/TUD data available.

5 Process or semi-empirical modelling

5.1 Introduction

For the empirical modelling of the removal of pathogenic micro-organisms and the formation of disinfection by-products by chlorination and ozonation, a literature study has been done. The purpose of this literature study was to find models, which describes the relation between the design and process parameters of a certain treatment process and the removal (or formation) of a certain water quality parameter.
In addition, several environmental parameters are considered which are directly or indirectly related to the removal or formation of the above mentioned parameters.

The following treatment processes are considered:
- Disinfection by chlorine
- Disinfection by ozone

The following parameters are considered:
- *Giardia*
- *Cryptosporidium*
- Enteroviruses
- Bromodichloromethane
- Trichloroacetic acid
- Temperature
- Dissolved organic carbon
- Acidity (pH)
- Bromide

5.2 Chlorination

5.2.1 Modelling the HOCl/OCl^--equilibrium

The HOCl/OCL^--equilibrium plays an important role in disinfection with chlorine. This is due to the fact that the disinfecting power of HOCl is much larger than that of OCl^-. The pH is an important factor in the location of the equilibrium. Modelling the effect of the HOCl/OCL^--equilibrium is derived from the classical Chick-Watson approach:
$\ln(N/N_0) = -k.CL_2^n.ContTime.$

In the case of a HOCl/OCl^--solution the final formulae is
$^{10}\log(N/N_0) = -k.\log e.ContTime.(CL_2/((H^+)+K_a))^n.((H^+)^n+a.K_a^n)$, in which K_a is a function of temperature (Haas, 1990): $\ln K_a = 23.184-0.0583(Temp+273.15)-6908/(Temp+273.15)$

(H^+)	H^+-concentration ($mol.l^{-1}$)
(HOCl)	HOCl-concentration (mg/l free chlorine)
(OCl^-)	OCl^--concentration (mg/l free chlorine)
a	relative disinfection efficiency
Cl_2	total free chlorine concentration (mg/l)
ContTime	contact time (min)
k	disinfection rate constant ($mg^{-n}.l^n.min^{-1}$)
K_a	association constant (mol/l)

N	concentration micro-organisms (number/l)
n	dilution coefficient
N_0	concentration micro-organisms on time 0 (number/l)
Temp	temperature (°C)

5.2.2 *Giardia*

In modelling *Giardia*, a choice can be made from a number of articles of good quality. In Leahy et al. (1987), experimentally determined Ct99-values (Ct-values giving 99 % inactivation) for *G. muris* for 3 pH's en two temperatures are presented; Further a Ct99-analysis is made of *G. lamblia*-data of other researchers. In the complex of articles of Clark (1990), Clark and Regli (1993), Clark et al. (1989, 1990) and Smith et al. (1995) an empirical model is presented, incorporating the model of Chick-Watson and the variables temperature, pH, chlorine concentration and contact time. The parameters were determined using various articles with data on the influence of these variables. In Haas and Heller (1990) the models of Chick-Watson, Selleck and Hom were compared using experimental data on *G. lamblia*, for three pH's and three temperatures, concluding that the model of Hom describes the data best. The parameters of the model of Hom at different pH's and temperatures are given.

It was decided to base the modelling in first instance on the complex of articles of Clark (1990), Clark and Regli (1993), Clark et al. (1989, 1990) and Smith et al. (1995), as in these articles the largest number of variables (temperature, pH, chlorine concentration and contact time) is taken into consideration. Leahy et al. (1987) restricted themselves to Ct-modelling. Haas and Heller (1990) did use the more flexible model of Hom, but they did not model pH and temperature. Within the complex of articles mentioned above the most recent article, that of Smith et al. (1995) was chosen.

From Smith et al. (1995) it is not clear what C exactly is: the dose, the rest concentration or something different. A conservative approach is to assume that it is the restconcentration: Cl_2 = Cl_2-Rest.
In the equation depends the removal of *Giardia* on the initial and the rest concentration of chlorine, the contact time, the temperatue and the pH. There is an equation for temperatures below and one for temperatures above 12.5 °C.

5.2.3 *Cryptosporidium*

The module for *Cryptosporidium* is based on Korich et al. (1990) who use the Ct-concept. In chlorine free water (which implies in principle a constant chlorine concentration) a Ct99-value was measured of 7200 mg.min.l^{-1} which leads to a value for k of $6.396.10^{-4}$ $l.mg^{-1}.min^{-1}$. This concept can be extended to a temperature correction and a correction can be applied for the HOCl/OCl^- equation.

If in the experiments of Korich et al. (1990) the chlorine concentration is indeed constant, in principle the above value for k can be used in a model formulation in which the concentration chlorine decreases exponentially. This leads to replacing the factor Cl_2 with the expression Cl_2 Dose($e^{-v.Time}$-1). The considerations above lead to an equation in which the course of the Cl_2 concentration, contact time, temperature and pH play a role.

5.2.4 Enterovirus

In Medema and Theunissen (1996), Sobsey et al. (1991) is used. Their Ct99.99-values are given for 3 pH's.

pH	Ct ($mg.l^{-1}.min$) (free available chlorine)
6	2.3
8	2.0
10	19.3

On the basis of these data the inactivation was modelled according to the Ct-approach, extended with the Q10-approach for temperature.

In the literature it was concluded that the model of Chick-Watson satisfies the best.

$$\log(EntvirOut/EntvirIn) = -k.Cl_2.ContTime.2^{(Temp-5)/10}\log e$$

The Chick-Watson-parameters (k, n) are given for 2 pH's and four temperatures.
For the effect of pH, the equation which uses the $HOCl/OCl^-$-equilibrium, is used. For viruses n=1 en a=0.004 in this equation (Chang, 1971). For experimental data Sobsey et al. (1991) is used. A conservative approach is used which implies that from the three Ct-values at different pH's given there the most conservative value is chosen as starting value for the calculations, with which the value of k is calculated. It can be reasoned that the Ct-waarde at pH=6 is the most conservative one and this one was used in first instance for modelling. The value of k was calculated using the $HOCL/OCL^-$-equations and equals 4.0735 $mg^{-1}.l.min$. During validation in a later stage it appeared that this value could not be maintained and it was calibrated for the situation in practice to 0.212 $mg^{-1}.l.min^{-1}$.
In summary, the model is extended with a factor $((H^+)+a.K_a)/((H^+)+K_a)$, in which k = 0.212 $mg^{-1}.l.min^{-1}$, a=0.004 and
$\ln K_a = 23.184-0.0583(Temp+273.15)-6908/(Temp+273.15)$

In the experiments of Sobsey et al. (1991) the mean of the initial and final concentration is used for the concentration of chlorine. We must choose here for incorporation in a model in which the rest concentration is used or a model in which the decrease in concentration is incorporated. The mean as a measure for concentration implies that translation to rest concentration gives a larger underestimation for the disinfecting action than translation to a "decrease model". This is why the last option is chosen.

The final formulae then becomes analogous to the equation for *Cryptosporidium.*

5.2.5 Trichloromethane

Three relevant articles were found on the formation of tricholoromethane (TCM or chloroform) is subject namely of Alekseeva et al. (1987), Clark et al. (1996) and Singer (1993). Alekseeva et al. (1987) presented an empirical model with variables COD, pH, chlorine concentration and contact time, using also the interaction terms between these variables. In Clark et al. (1996) the variables pH, time, chlorine- and bromide concentration were considered. Singer (1993) presents a model in which all variables are risen to a power and subsequently multiplied with each other. The variables are TOC (total organic carbon) and UV-254 (absorption of ultraviolet light at 254 nm) (both as surrogate parameters for disinfection by-products (DBP- precursors), pH, chlorine dosis, contact time, temperature and bromide concentration.

In summary, all these authors incorporated pH, chlorine concentration and contact time in their modelling. Only Singer (1993) used in addition temperature and therefore this model will be applied here. The model of Singer (1993) contains three variables (TOC, UV-254 and bromide) that were in first instance not incorporated in the first fase of TAPWAT. Assuming that there is hardly a difference DOC is substituted for TOC in the model of Singer (1993). For the values of UV-254 and bromide, an estimation was made on the basis of REWAB-data (mean values) for the years 1992 up to and including 1995 for Andijk, Rotterdam-Beerenplaat, Rotterdam-Kralingen and Amsterdam-Leiduin. The mean of intake and finished water should be considered as an estimation of the water quality of the oxidation process, which is situated somewhere between intake and finished water. The resulting values are:

- UV-254 = 0.0655 cm^{-1}
- bromide = 0.1635 mg/l

Not incorporating bromide was in addition justified by an analysis of the minimum- and maximum values in the years and for the purification plants mentioned above. Substitution of the lowest and highest values found (0.050 en 0.52 mg/l) in the model of Singer (1993) gives a ratio between extreme TCM_{out}-values of 2.3. This can be compared with an a priori acceptable ratio of 5 (pers.comm. Versteegh), which justifies not incorporating bromide in the model equation.
This leads to the following equation:

$$TCMOut = k1 \cdot DOC^{k2} CL2\_Dose^{k3} ContTime^{k4} Temp^{k5} (PH - k6)^{k7}$$

with k1 = 0.037 (complexe dimensie), k2 = 0.616, k3 = 0.391, k4 = 0.265, k5 = 1.15, k6 = 2.6, k7 = 0.800 and

TCMOut = Trichloromethane concentration in outflow (µg/l)
DOC = Dissolved Organic Carbon (mg/l)
CL_2 dose = Dose chlorine concentration (mg/l)
ContTime = Contact time (hours)
Temp = Temperature (°C)
PH = pH

5.2.6 Bromodichloromethane

For chlorination and the formation of bromodichloromethane (BDCM) the situation is analogous to chlorination and the formation of trichloromethane, the only difference being that Alekseeva et al. (1987) did not work on bromodichloromethane.

In the model of Singer (1993) is substituted UV-254 = 0.0655 cm^{-1}, Bromide = 0.1635 mg/l and DOC for TOC.
Not incorporating bromide is justified by an analysis analogous to trichloromethane which gives a ratio between extreme $BDCM_{out}$-values of 1.3 which in turn justifies not incorporating bromide in the model equation.
The equation is analogous to that for trichloro methane with TCM_{Out} replaced by $BDCM_{Out}$ (Bromodichloromethane in outflow (µg/l)). The parameter values are:
k1 = 0.594 (complex dimension), k2 = 0.177, k3 = 0.309, k4 = 0.271, k5 = 0.720, k6 = 2.6, k7 = 0.925.

5.2.7 Trichloroacetic acid

For chlorination and the formation of trichloroacetic acid (TCA) the situation is analogous to chlorination and the formation of trichloromethane, the difference being that Alekseeva et al. (1987) did not work on TCA and that the model of Singer (1993) does not incorporate temperature for this compound. Further, TOC and UV-254 are not in the formula for TCA as a product, but as separate variables.

In the model of Singer (1993) is substituted UV-254 = 0.0655 cm^{-1}, Bromide = 0.1635 mg/l and DOC for TOC.
Not incorporating bromide was justified by an analysis analogous to trichloromethane which results in a ratio between extreme TCA_{out}-values of 1.3 which in turn justifies not incorporating bromide in the model equation.
This leads to the following equation:

$$TCAOut = k1 \cdot DOC^{k2} CL2\_Dose^{k3} ContTime^{k4} pH^{k5}$$

TCAOut = Trichloroacetic acid in outflow(µg/l)

For a description of the other variables one is referred to trichloromethane.
k1 = 73.4 (complex dimension), k2 = 0.355, k3 = 0.881, k4 = 0.264, k5 = -1.732. As a result of calibration, it proved necessary to replace the original value of k1 (based on the work of Singer) with the value above.

5.2.8 Verification of formation of trichloromethane by chlorination

In paragraph 5.2.5 the formulae for the prediction of the formation of trichloromethane are summarised.

For the prediction of trichloromethane formation by chlorination the adapted model of Singer (1993) is used:

$$TCM_{out} = 0.037 * (TOC)^{0.616} * Cl_2 dose^{0.391} * ContTime^{0.265} * Temp^{1.15} \ldots$$
$$* (pH - 2.6)^{0.8}$$

where,

TCM_{Out}	= Trichloromethane concentration in outflow (µg/l)
TOC	= Total Organic Carbon (mg/l)
CL_2 dose	= Chlorine dose (mg/l)
ContTime	= Contact time (hours)
Temp	= Temperature (°C)
pH	= pH

Data from WNWB-Zevenbergen and PWN-Andijk are used for the validation of this formula. At these plants chlorination takes place for disinfection purposes. The results are shown in the figures 5.1 and 5.2.
Visual interpretation of the graph leads to the conclusion that the prediction of the formation of trichloromethanes at Zevenbergen is rather good, in accordance to the prediction of the first year at Andijk. The results of the second year at that pumping station give a high overestimation of practice. This is mainly due to the fact that in this period sodiumbisulfite is

dosed at the end of the contact tanks, which takes out the chlorine and thus reduces the contact time and consequently the formation of trichloromethanes.

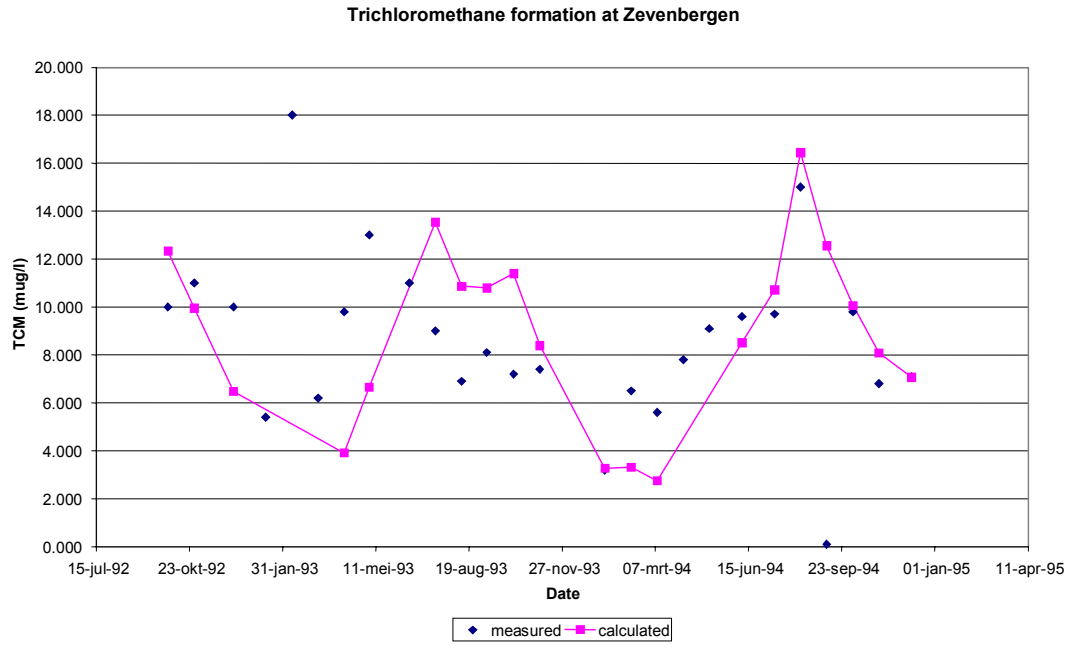

Figure 5.1 Example 1 of a validation of the module chlorination

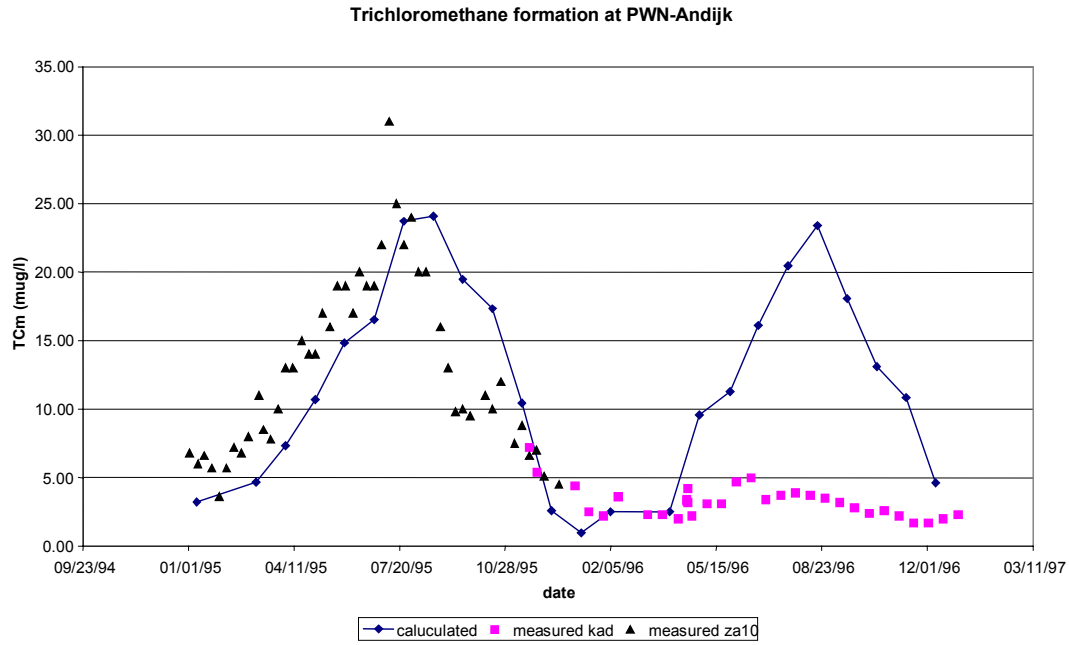

Figure 5.2 Example 2 of a validation of the module chlorination

Further it can be concluded from the data of PWN-Andijk (and Zevenbergen) that there is a retardation in the prediction. It is uncertain which is the cause of it, but for the model TAPWAT this is not relevant. It is mainly of importance that a certain concentration peak is predicted and the exact time of the occurrence not.

5.3 Ozonation

5.3.1 *Giardia*

In Medema and Theunissen (1996), the data of Finch et al. (1993a) are used. In there the inactivation was determined for a range of five Ct values. Based on these data, the inactivation was modelled according to the Ct-concept, extended with the Q10 approach for temperature.

Finch et al. (1993a) calculated parameters of the model of Hom. This application of the model of Hom was coupled to the assumption of an exponential decrease of the ozone concentration with time. This is a somewhat curious approach, as a very empirical equation is combined with a process description approach. Therefore it was decided to perform an analogous calculation of the parameters of the model of Hom as in Finch et al. (1993b) in order to apply this model in the first phase of TAPWAT.

Finch et al. (1993a) used the ozone residual for the ozone concentration for an analysis of the data according to the Ct-concept; For this reason this will be done also in this model formulation (OZ = OZ-rest). At least squares fitting was done with the model of Hom and the data of Finch et al. (1993a).

For TAPWAT the model of Hom, extended with a temperature correction, can be reformulated into the following equation.

$$GiardiaOut = GiardiaIn \cdot 10^{\frac{-k1 \cdot OZ\text{-}Rest^{k2} ContTime^{k3+1} 2^{\frac{Temp-k4}{k5}} \log e}{k3+1}}$$

met

k1	= Disinfection rate constant k	= 2.229 $mg^{-k2}.l^{k2}.min^{-(k3+1)}$
k2	= Dilution coefficient n	= 0.138(-)
k3	= Homcoefficient m	= -0.560 (-)
k4	= base temperature for temperature effect	= 22 °C
k5	= temperature rise for doubling the disinfection rate	= 10 °C
*Giardia*Out	= Concentration *Giardia* in outflow (number/l)	
*Giardia*In	= Concentration *Giardia* in inflow (number/l)	
OZ-Rest	= Rest concentration ozone (mg/l)	
ContTime	= Contact time (min)	
Temp	= Temperature (°C)	

5.3.2 *Cryptosporidium*

Medema and Theunissen (1996) used the data of Finch et al. (1993b). In there a large dataset on ozone inactivation of *Cryptosporidium* is presented. Based on these data the inactivation was modelled according to the Ct-concept, extended with the Q10 approach for temperature. Finch et al. (1993b) calculated the parameters of the model of Hom for two temperatures.

Finch et al. (1993b) used the so-called ‘integrated ozone residual’ as a measure for the ozone concentration. This is a geometric mean of initial and final concentration. The parameter

values calculated by Finch et al. (1993b) can be used for application of the model of Hom combined with exponentially decreasing disinfectant concentration. This model is not analytically solvable. Application of this model is possible using numerical integration. This modelling approach is somewhat curious however, as a very empirical formula is combined with a process description approach.

Therefore now the model of Hom is applied with a constant disinfectant concentration. For OZ the rest concentration is substituted (OZ = OZ-rest) and the formula is extended with a temperature correction. The parameters of Hom at 7 °C were used. The resulting equation is analogous to the equation for *Giardia*, with *Giardia*Out en *Giardia*In replaced by CryptoOut and CryptoIn, respectively, the concentration *Cryptosporidium* in outflow and inflow (number/ml). The parameter values are:

k1	= Disinfection rate constant k	= 0.634 $mg^{-k2}.l^{k2}.min^{-(k3+1)}$
k2	= Dilution coefficient n	= 0.68(-)
k3	= Hom coefficient m	= -0.05 (-)
k4	= base temperature for temperature effect	= 7 °C
k5	= temperature rise for doubling the disinfection rate	= 15 °C

5.3.3 Enterovirus

Medema and Theunissen (1996) used the data of Roy et al. (1980). In this article data are presented on well performed experiments on the effects of concentration, contact time, pH and temperature on the inactivation of poliovirus 1. Modelling was performed based on these data, using the Ct and the Q10 approach.

Herbold et al. (1989) determined the parameters of an exponential inactivation model at different ozone concentrations and temperatures for hepatitis A virus and poliovirus 1. As the model information in this article does not lead to improvement or extension of the model formulation, it was decided in first instance to apply the approach of Medema and Theunissen (1996).

In the experiments of Roy et al. (1980) the ozone concentration was kept constant during the exposure time using a continuous flow reactor. In this situation the value of k (see parameter list) can be determined. It equals 20.93 $mg^{-1}.l.min^{-1}$.. In principle this same value of k can be applied in a model formulation in which the concentration of ozone declines exponentially. However, from a validation procedure it appeared that this value had to be changed for the situation in practice to 0.799 $l.mg^{-1}.min^{-1}$. The above leads to the following model:

$$\text{EntvirOut} = \text{EntvirIn} \cdot 10^{\log_e\left(\frac{k1}{k4}\right)\text{OZ - Dose}\left(e^{-k4\cdot\text{ContTime}}-1\right)2^{\frac{\text{Temp}-k2}{k3}}}$$

k4 follows from the dose, rest concentration and the contact time, according to OZ_Rest = OZ-Dose.$e^{-k4.ContTime}$, so that

$$k4 = \frac{-\ln\left(\frac{OZ\text{ - }Rest}{OZ\text{ - }Dose}\right)}{ContTime}$$

k1	= Disinfection rate constant k	= 0.799 $l.mg^{-1}.min^{-1}$
k2	= base temperature for temperature effect	= 5 °C
k3	= temperature rise for doubling the disinfection rate	= 10 °C
k4	= Disappearing rate constant v (min^{-1})	
EntvirOut	= Concentration virus in outflow (number/l)	
EntvirIn	= Concentration virus in inflow (number/l)	
OZ_Dose	= Dose concentration ozone (mg/l)	
OZ_Rest	= Rest concentration ozone (mg/l)	
ContTime	= Contact time (min)	
Temp	= Temperature (°C)	

5.3.4 Bromate

On modelling bromate formation during ozonation two relevant articles were found. Schmidt et al. (1995) give a model with variables ozone, DOC and bromide. Song et al. (1996) modelled the variables bromide, DOC, ammonia-nitrogen, ozone, pH, alkalinity and reaction time. Because of the modelling of pH and reaction time, the model of Song et al. (1996) was chosen.

The model of Song et al. (1996) contains three variables (bromide, ammonia-nitrogen and alkalinity) that were in first instance not modelled in the first phase of TAPWAT. Therefore an estimation was made for the values of bromide, ammonia-nitrogen and alkalinity, using the same data and approach as for trichloromethane. For the calculation of alkalinity the formule in Schock (1990) was used:

- Total alkalinity = $(HCO_3^-) + 2(CO_3^{2-}) + (OH^-) - (H^+)$
- The resulting values are:
- bromide = 0.1635 mg/l
- NH_4-N = 6.5528 mg/l
- alkalinity = 215.5631 mg $CaCO_3$/l

The incorporation of bromide was further investigated by an analysis analogous to trichloromethane, which gives a ratio between extreme bromate concentrations of 7.9, which in turn implies that bromide has to be incorporated into the model formulation. This results in the following equation.

$$Bromate = k1 \cdot DOC^{k2} OZ\text{ - }Dose^{k3} PH^{k4} ContTime^{k5} Bromide^{k6}$$

with k1 = $1.46.10^{-6}$ (complex dimension), k2 = -1.18, k3 = 1.42, k4 = 5.11, k5 = 0.27, k6 = 0.88 and

Bromate	= Bromate (µg/l)
DOC	= Dissolved Organic Carbon (mg C/l)
OZ_Dose	= Dose ozone concentration (mg/l)
PH	= pH (-)
Alkalinity	= alkalinity (mg $CaCO_3$/l)
ContTime	= Contact time (min)
Bromide	= bromide (µg/l)
NH_3-N	= ammonia-nitrogen (mg N/l)

5.4 Conclusions

The formulae, presented in this chapter, are based on many observations. The validation for Dutch circumstances only is tested. As can be seen in paragraph 5.2.8, this is done for the formation of trichloromethane after chlorination.
In TAPWAT the modules chlorination and ozonation are incorporated for the prediction of disinfection by-products.
The result of the empirical models is a point estimate for the formation of disinfection by-products and the distribution in the input data will therefore directly be transferred to the output. No extra uncertainty is introduced in this module.

6 Stochastic modelling of the removal of natural organic compounds in drinking-water processes

6.1 Introduction

In the preceding chapters, the removal and formation of compounds and the removal of organisms is determined by empirically determined removal percentages (and ranges) and by point estimates based on regression analyses of the performance of treatment plant in the USA.

The disadvantage of point estimates is that it is not clear what is the confidence interval of the calculated value. In design and operation of modern drinking-water production processes it is necessary to perform probabilistic modelling. As formulated by Haarhoff (Haarhoff, 2000): *"For models that will be increasingly used for optimization, it is essential that predictions are formulated in probabilistic terms. Designers and operators need not only know the average performance of a process, but are specifically interested in the tails of the performance distribution, as good performance has to be maintained under extreme conditions. This requirement becomes quite evident when the performance of a system has to be predicted, given the performance of the individual processes making up the system".*

With test data statistical techniques are used to construct an appropriate model and to estimate its parameters. Once a model is obtained, it may, of course, be used to predict future performance (Hahn, 1967).

For the determination of the statistical distribution of removal percentages by a specific process, different models can be used.
For the removal or organic compounds the "beta-distribution" is chosen, because of its continuous character and its flexibility in shape in the range between 0 and 1 (0-100%).

6.2 Removal of organic compounds in conventional drinking-water treatment processes

In conventional treatment plants natural organic compounds are only removed by floc formation/removal and by activated carbon (filtration).
NOM may cause colour, is a precursor for disinfection by-products, can compete with adsorption sites for pesticides and VOC's (Kruithof 1994; Sorial, 1994; Summers, 1993, Hopman, 1991) and can promote microbial growth and fouling of membranes.

Floc formation and removal.
Dennet (Dennet, 1996) reviewed several articles and did some research (jar-tests) on concentrated river and lake water. The effectiveness of coagulation for removing NOM depends on charge, solubility and molecular-size characteristics. The efficiency of removing organic carbon is proportional to molecular size, with larger-molecular-weight components more effectively removed than smaller ones. Sinsabaugh (Sinsabaugh, 1986) determined that acidic and basic components of the NOM in natural waters were twice as likely to be removed by coagulation as non polar neutral compounds. The removal of neutral compounds depended on their polarity and the availability of low-polarity sorption sites on the floc. (Phylic and phobic compounds were precipitated more readily than mesics).

Coagulation depends primarily on the pH (lower than for turbidity removal: 4-5), coagulant dosage(proportional to NOM concentration) and NOM concentration.
From the experiments it was concluded that water with high concentrations of humic and fulvic acids is better coagulated (85-95%) removal than water with mainly amino acids, sugars, various aliphatic and aromatic acids and other organics (15-35% removal).
Hubrec (Hubrec, 1992) suggested that NOM in the form of TOC and DOC is removed by coagulation with a percentage of <60% and 25-40% respectively.

Activated carbon filtration
A first indication of the possible removal of NOM by granular activated carbon is given with the Freundlich-isotherm. This equation determines the adsorption capacity of activated carbon for a certain compound (Hopman, 1991).
The Freundlich-isotherm is given by:

$$q = K \cdot c_{equil}^{\,n}$$

where: K = constant [(g/kg)·(m3/g)n]
n = constant [-]
c_{equil} = equilibrium concentration [g/m3]
q = adsorption capacity [g/kg]

Compounds that adsorb easily have a high value of K (Kruithof, 1994).
The value of K increases in the following cases:
- Increase in molecular weight;
- Substitution with halogens;
- Increase in the number of double bounds.

The value of K decreases in case of substitution with polar groups such as COOH and OH.
Pesticides that are polar will be removed less than pesticides that are a-polar.
A low value of n means that the adsorption capacity is less depend on the concentration in the liquid.

When several organic compounds are present in the water, adsorption of compounds with the highest K-value is predominant. It can even occur that a certain compound desorbs because another, better adsorbable compound is present in the water.
The content of Natural Organic Matter determines heavily the removal of organic micro-pollutants (like pesticides) by activated carbon filtration. When NOM is adsorbed adsorption places for the removal of pesticides are occupied and an early pesticide breakthrough will occur. NOM will also block the pores, with as consequence that the internal pores are no longer available for adsorption (Hopman, 1991).

The type of carbon that is used determines the removal efficiency. The specific behaviour of a type of activated carbon is determined by:
- surface area and pore structure; Adsorption of pesticides takes place in the micro pores of the activated carbon. The larger the specific surface area is the better will in general the adsorptive capacity be. But when water contains a relatively large NOM-content the NOM will block the micro pores and the adsorption capacity will drop. For polar compound activated fibre carbon is used. This carbon has a pore structure with only micro pores, resulting in less blocking and a larger adsorption velocity.

- particle size; the surface area increases with a decrease in particle size, resulting in a higher adsorption capacity.

The equilibrium will change with a changing temperature. An increase in temperature will result in a decrease of adsorption capacity. When the initial concentration is low this effect is more pronounced than with higher initial concentrations.

When the influent concentration is constant the effluent concentration of NOM will increase in time (breakthrough curve). After reaching a pre-set concentration the filter will be regenerated.

Interaction between coagulation and activated carbon filtration (Semmens, 1986)
Coagualtion can remove a large fraction of the NOM's in river water. Coagulation pretreatment of river water improves the performance of GAC for TOC and THM precursor removal. The improved removal of organics after pretreatment is thought to be due to the combined effects of reduced influent TOC and the removal of poorly adsorbed higher-molecular-weight organics.

6.3 Beta-distribution

The beta probability density function defined over the interval (0,1) is (Hahn, 1967):

$$f(x;\gamma,\eta) = \frac{\Gamma(\gamma+\eta)}{\Gamma(\gamma)\Gamma(\eta)} x^{\gamma-1}(1-x)^{\eta-1}, \quad 0 \le x \le 1, \quad 0 < \gamma, \quad 0 < \eta$$

The maximum likelihood estimates of the beta-distribution parameters are given by the following equations:

$$\eta = \frac{(1-\mu)}{\sigma^2}[\mu(1-\mu)-\sigma^2]$$

$$\gamma = \frac{\mu\eta}{(1-\mu)}$$

$$\mu = \frac{\sum x}{n}$$

$$\sigma^2 = \frac{n\sum x^2 - (\sum x)^2}{n(n-1)}$$

In the Statistics Toolbox of Matlab the following functions are available for the determination of the distribution: Betafit, Betapdf, Betastat.
With the first function the parameters η and γ for the beta-distribution can be determined. With the second function the distribution Y can be calculated, using X-data and the parameters η and γ. With the last function the mean μ and the variance σ^2 of the distribution can be calculated.
The relations between the parameters η, γ and μ and σ^2 can also be written as:

$$\eta = \frac{1-\alpha^2}{\alpha^2}(1-\mu)$$

$$\gamma = \frac{1-\alpha^2}{\alpha^2}\mu$$

where

$$\alpha^2 = \frac{\sigma^2}{\mu(1-\mu)}$$

The beta-distribution can only cope with data between 0 and 1 and therefore the removal percentages are divided by 100. When negative data occur, they are skipped.

6.4 Distribution of removal of Total Organic Carbon by floc formation and removal

For the modelling three treatment plants are analysed. The designs of the three treatment plants are definitely different and this will influence the performance of floc formation and floc removal. A summary is given in table 6.1.

Table 6.1 Characteristics of coagulation process of three treatment plants in the Netherlands

	Coagulant	Dose	Floc removal	pH settled water
WRK III	$Fe_2(SO_4)_3$	20 mg Fe/l	Tilted plate settling	7.7
WNWB	$FeCl_3$	8 mg Fe/l	Flotation	7.95
WRK I-II	$FeCl_3$	3 mg Fe/l	Horizontal flow settling	7.2 (8.2)

For the determination of the beta-distribution for the removal of TOC by floc formation and floc removal, the following data are used:
65 removal percentages of WRK III (4 negative values thrown away)
52 removal percentages of WNWB
223 removal percentages of WRK I-II (1 negative value thrown away)

Table 6.2 Results of calibration "beta-distribution" TOC removal by floc formation and removal

	η	ηint	γ	γint	μ	σ^2	α
WRK III	7.44	6.3-8.6	15.25	12.3-18.2	0.328	0.0093	0.21
WNWB	8.63	4.5-12.8	28.08	14.4-41.8	0.235	0.0048	0.16
WRK I-II	7.92	6.8-9	22.62	19.4-25.8	0.259	0.0061	0.18

Because WRK III has a higher coagulant dose, the removal of organic carbon is higher than with the other plants.
It can be observed that the interval of η and γ of plant WNWB is wider than the others.
With the value of μ being specific for each plant and the average value α (α=0.195) for the plants WRK III and WRK I-II, the frequency distribution is determined.
In figure 6.1 the results are represented.

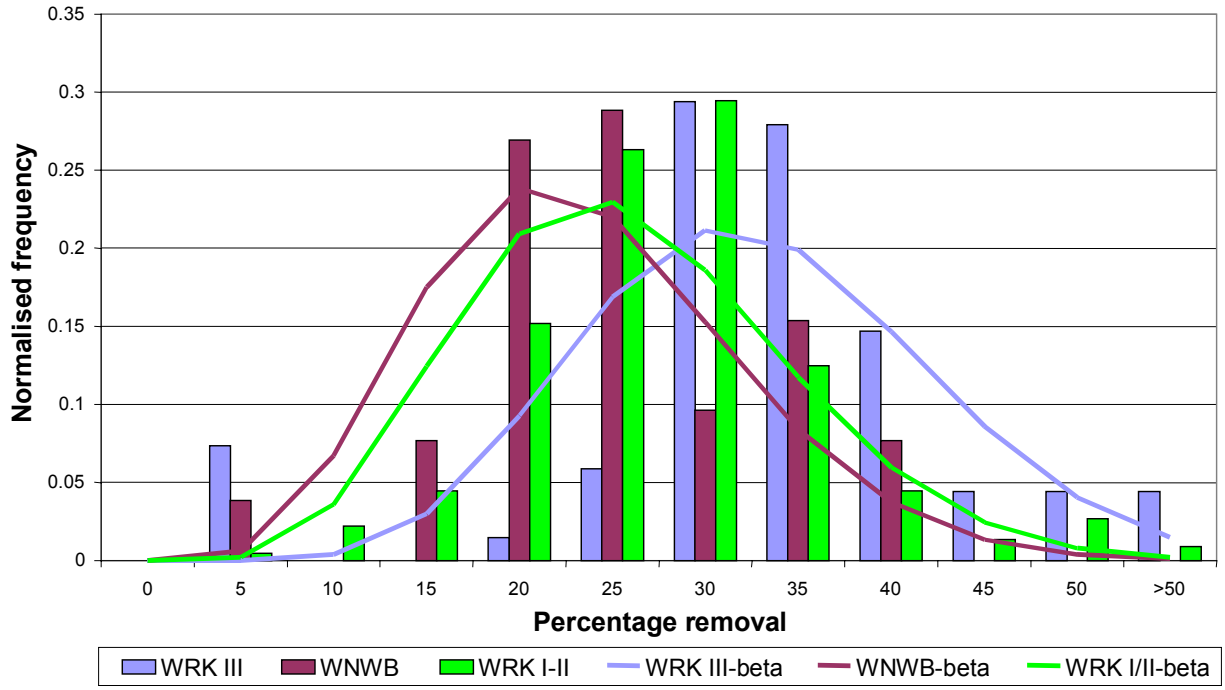

Figure 6.1 Beta-distribution for the removal of TOC by coagulation at three treatment plants

6.5 Distribution of removal of Total Organic Carbon by activated carbon

Activated Carbon Filtration (GAC) has an effect on the removal of dissolved organic carbon through adsorption processes. This process will go on and gradual break-through will occurr until the carbon is saturated and must be regenerated.

For the modelling two treatment plant are analysed. These plants have different removal capacities and reasonable spreading of the percentages occur. This is due to differences in influent level and differences in the design. In addition, the different filters are rotatively regenerated and the effluent quality will be levelled off, depending on the number of filters present in the installation. A summary of the characteristics of the filters is given in table 6.3.

Table 6.3 Characteristics of GAC process of two treatment plants in the Netherlands

	EBCT (min)	no. filters	Regeneration	pre-oxidation	TOC influent (mg/l)
WRK III	12.5	8 (70*1.8m2)		-	4
WNWB	25	3 (58.3m3)	18000BV	Cl2	2.64

For the statistical analysis of activated carbon filtration data of two plants are used: WRK III and WNWB.
The flow through the filters can not exactly be determined:

- The intake flow can be higher than the treated flow due to losses (backwash)
- The intake flow of WNWB is not exactly know on the data of the sampling, but flows from several days later or earlier are taken

- The filtration flow of WRK III is not exactly known, because only part of the total flow is filtered through the GAC. Here it is assumed that globally half (0.5) of the total flow is filtered.

For the determination of the beta-distribution for the removal of TOC by activated carbon filtration
The following data are used:
77 removal percentages of WRK III (15 negative values thrown away)
58 removal percentages of WNWB

Table 6.4 Results of calibration "beta-distribution" TOC removal by activated carbon filtration.

	η	ηint	γ	γint	μ	σ^2	α
WRK III	1.723	1.3-2.1	8.931	6.9-11	0.162	0.0116	0.29
WNWB	4.978	3.12-6.8	6.7	4.22-9.21	0.426	0.0193	0.28

Because WNWB has only three filters the performance will fluctuate more than with the other plants. The EBCT of WNWB is higher (and in combination with the chlorination) this will result in a good performance.
With the value of μ being specific for each plant and the average value α (α=0.285), the frequency distribution is determined.
In figure 6.2 the results are represented.

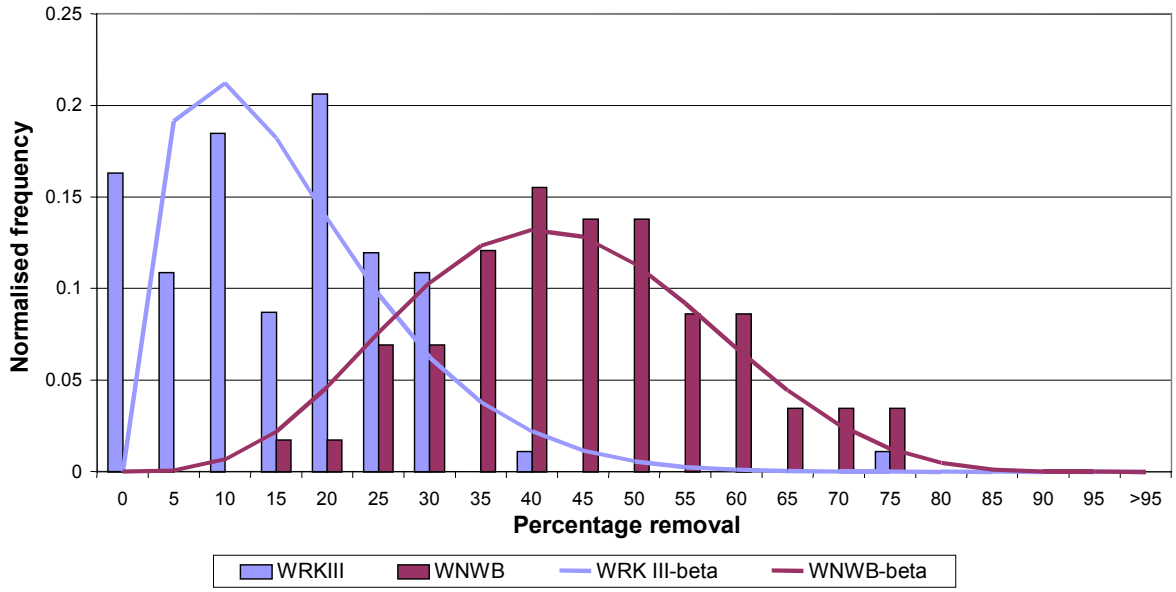

Figure 6.2 Beta-distribution for the removal of TOC by GAC at two treatment plants

6.6 Conclusions

It can be concluded that the percentages of removal of TOC by coagulation and granular activated carbon (GAC) can be described by the beta-distribution.
For every plant the distribution is different, because of differences in design and in influent water characteristics. However, here (after some manipulations) it was concluded that value α

is more or less constant for a specific process. When the value of μ for a specific plant is known, the beta-distribution can then be determined. Value μ is the equivalent for the average removal ratio of TOC by the treatment process. In this chapter only a few plants are analysed and therefore it is not possible to compose general expressions for the estimation of value μ. This could be the case when more plants are analysed in the same way.

Assuming that the different parameters, influencing the removal ratio of the treatment process, are independent of each other, the beta-distribution can be used for Monte-Carlo analysis of the treatment processes.

7 Validations and applications of TAPWAT

7.1 Introduction

In this chapter a number of validation steps will be described that have been performed with TAPWAT. The emphasis in these descriptions will be on the meaning of the results for the use and further development of the model TAPWAT itself. The following validations and applications will be treated:

- Validation on the basis of data from the practice of drinking-water companies;
- Application for balancing the risks of micro-organisms and disinfection by-products.

It would be beyond the pale of this report to show all the results of the calculations concerned, therefore representative examples of these results will be shown.

7.2 Validation of TAPWAT based on company data

Large amounts of information have been collected consisting mainly of measurements made by several drinking-water companies. With this information validations were performed with the available modules as part of a complete treatment system. Use was made of the Monte Carlo method to indicate the uncertainty of the results.

7.2.1 Basic assumptions

The calculations have been based on the data collected from the drinking-water companies; this goes for the quality of the raw water and the values of design and process parameters. Monte Carlo analysis has been applied with 250 draws for every time step (see paragraph 3.5 for a description of Monte Carlo analysis).

Based on this input, results for a number of existing treatment systems have been calculated, using the process modules for ozonation and chlorination. Added to this were modules consisting of a range of removal percentages instead of the single percentage. The results have been compared to data concerning the quality of drinking water, also supplied by the drinking-water companies.

7.2.2 Example of the results

As an example the results will be shown concerning the following treatment system:

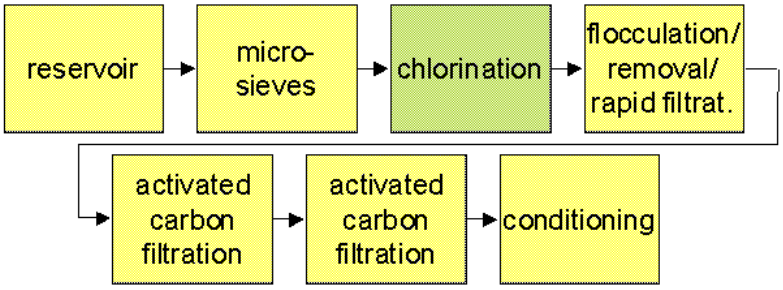

Figure 7.1 Example treatment system of the calculations based on company data.

The treatment steps indicated green have been represented during the calculations by process modules, the other steps by modules consisting of a range of removal percentages.

In figure 7.2 the results are shown for atrazin over the years 1995-1996. The small number of available measurements in drinking water were all under the detection limit of 0.05 µg/l; represented in the graph is half the detection limit. Based on these scanty facts, the concentration of atrazin seems to be calculated reasonably well. But in fact the validation is very weak because of te very few data. To do this in a better way more data are needed from a system where concentrations slightly above detection limt are measured. Finished drinking water is not suitable for validation of this model because measurements always gives data around the detection limit because of the existing standard (0.1 µg/l) in drinking water.

The graph in figure 7.3 represents the calculated and measured concentration of TOC (Total Organic Carbon). Here, the calculations and measurements match rather well. However, the range of the calculated values is more than the dispersion of the measured ones.

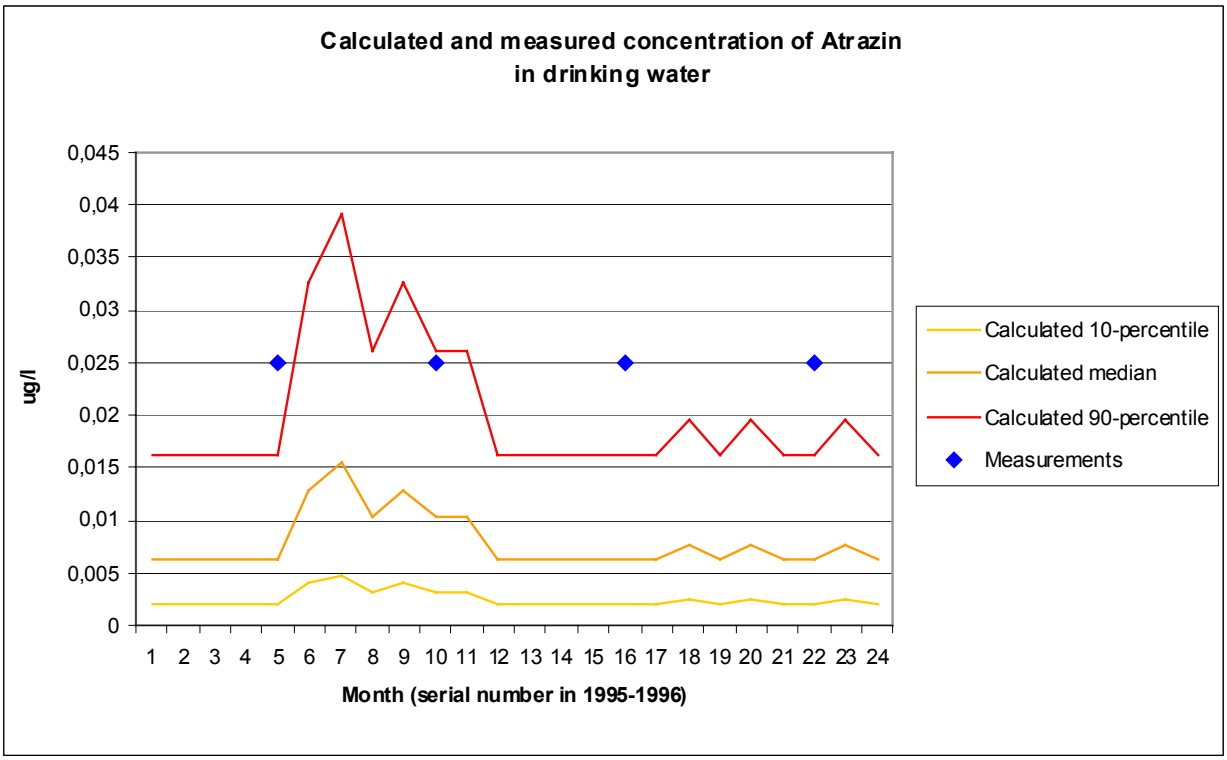

Figure 7.2 Calculated and measured concentration of atrazin in drinking water over the years 1995-1996. Measurements were all below detection limit (0.05 µg/l).

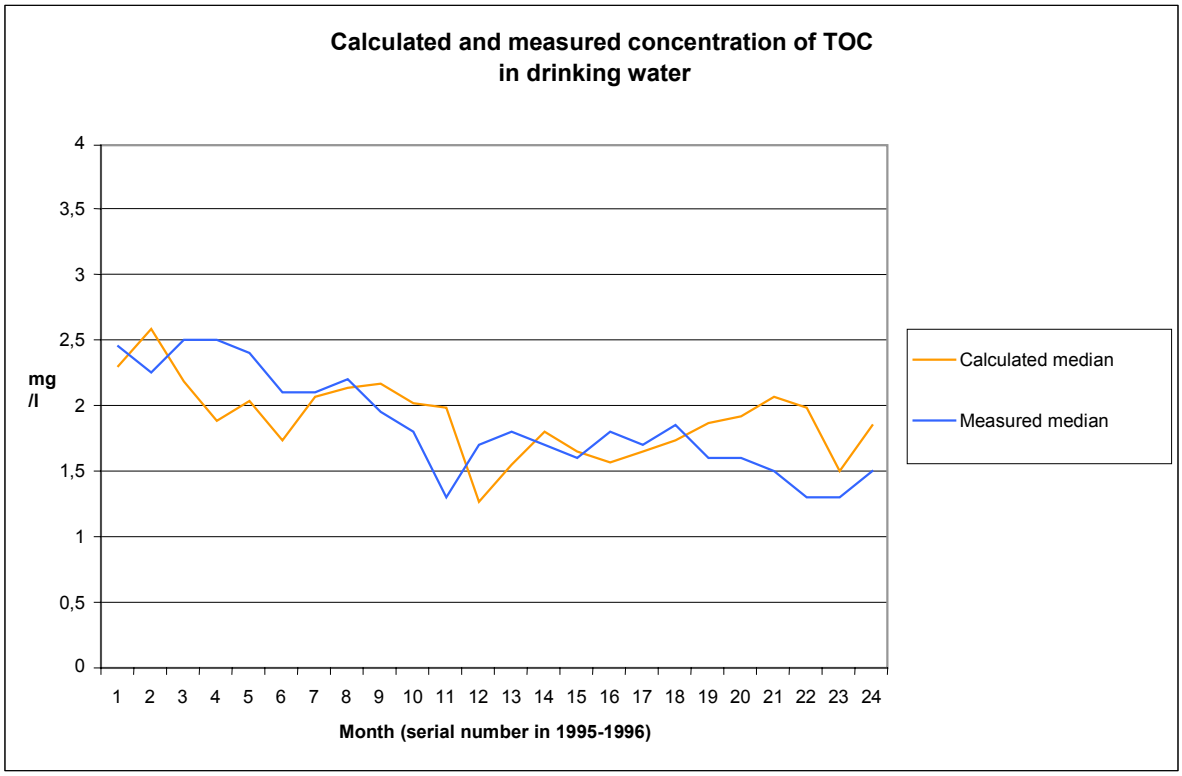

Figure 7.3 Calculated and measured concentration of TOC in drinking water over the years 1995-1996. Monte Carlo analysis is not shown.

7.2.3 Conclusions

The following conclusions can be drawn from the validations on the basis of company data:

- Over the two-year period concerned, the dispersion of the calculated values is more than the dispersion of the measurements. This seems to indicate that the assumption, as used in the Monte Carlo analysis, of an even distribution of the values of input items between the minimum and maximum of the given range, is not correct. This is also the reason why Monte Carlo is not used in figure 8.3. Tests are needed with draws based on other distributions.
- The modules in TAPWAT are based on an average performance of a treatment step; this can differ from the performance of a step in a particular treatment system. Caution is necessary in applying the model on specific cases.

7.3 Balancing the risks of micro-organisms and disinfection by-products as an application

As an example of how to use TAPWAT for determining the treatment system needed to produce drinking water from surface water with the quality of the IJsselmeer, calculations have been made for balancing the risks of micro-organisms and disinfection by-products.

7.3.1 Basic assumptions

Three possible treatment systems have been analysed:

- A system with ozonation, which will remove the micro-organisms but produces the by-product bromate;
- A system with soil passage, removing the micro-organisms;
- A system without ozonation and without soil passage.

These three systems are shown in figure 7.4; treatment steps indicated green were represented by process modules, the other steps by modules consisting of percentage ranges.

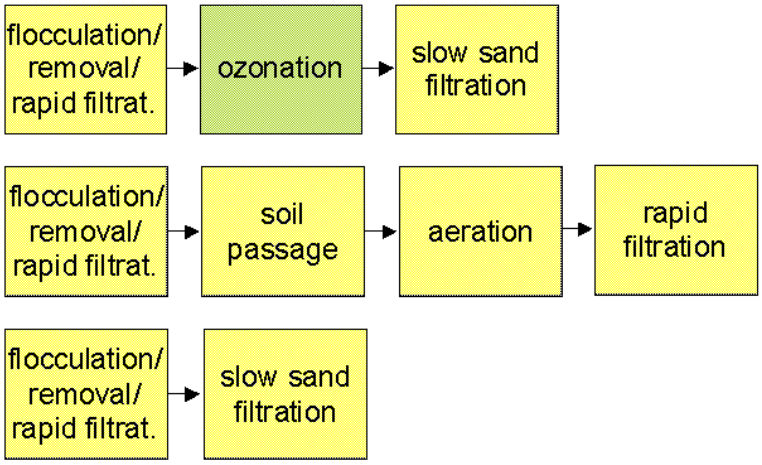

Figure 7.4 The three treatment system as analysed in balancing the risks of micro-organisms and disinfection by-products. The first system corresponds with the blue line (with ozone) in figure 7.5; the second system with the green line (with soil passage) and the last system corresponds with the black line (without ozone) in figure 7.5.

This means that the future amounts of micro-organisms in raw water were based on results of the model WATNAT. Other information concerning raw surface water that was required by TAPWAT, such as pH, DOC, temperature and concentration of bromide, was based on the present quality of surface waters as available in information system ISDIV.
For the ozone step the modelparameters are contact time 24 minutes; ozone dose 1.75 mg/l; rest ozone 1.25 mg/l. For soil passage the reduction of *Cryptosporidium* is 3 log units and for slow sand filtration it is ca. 3 log units

The risk level for *Cryptosporidium* is derived (Teunis et al.) from the global risk level for diarrhoea for the Netherlands of 1 case per 10,000 inhabitants per year caused by drinking water.

7.3.2 Results

In figure 7.5 the calculated amounts of *Cryptosporidium* in drinking water are shown, as compared with the risk level of $2.6*10^{-5}$ oocysts/litre. The graph shows that the drinking water produced by the treatment system without ozonation contains amounts of *Cryptosporidium* way slightly above the risk level. The treatment system with soil passage yields better results; however, the levels of *Cryptosporidium* are slightly below the risk level. The treatment system with ozonation produces drinking water with acceptable amounts of *Cryptosporidium,* however the levels are extremely low. The pattern troughout the year shows also the pattern in the source for the production plant (river water).

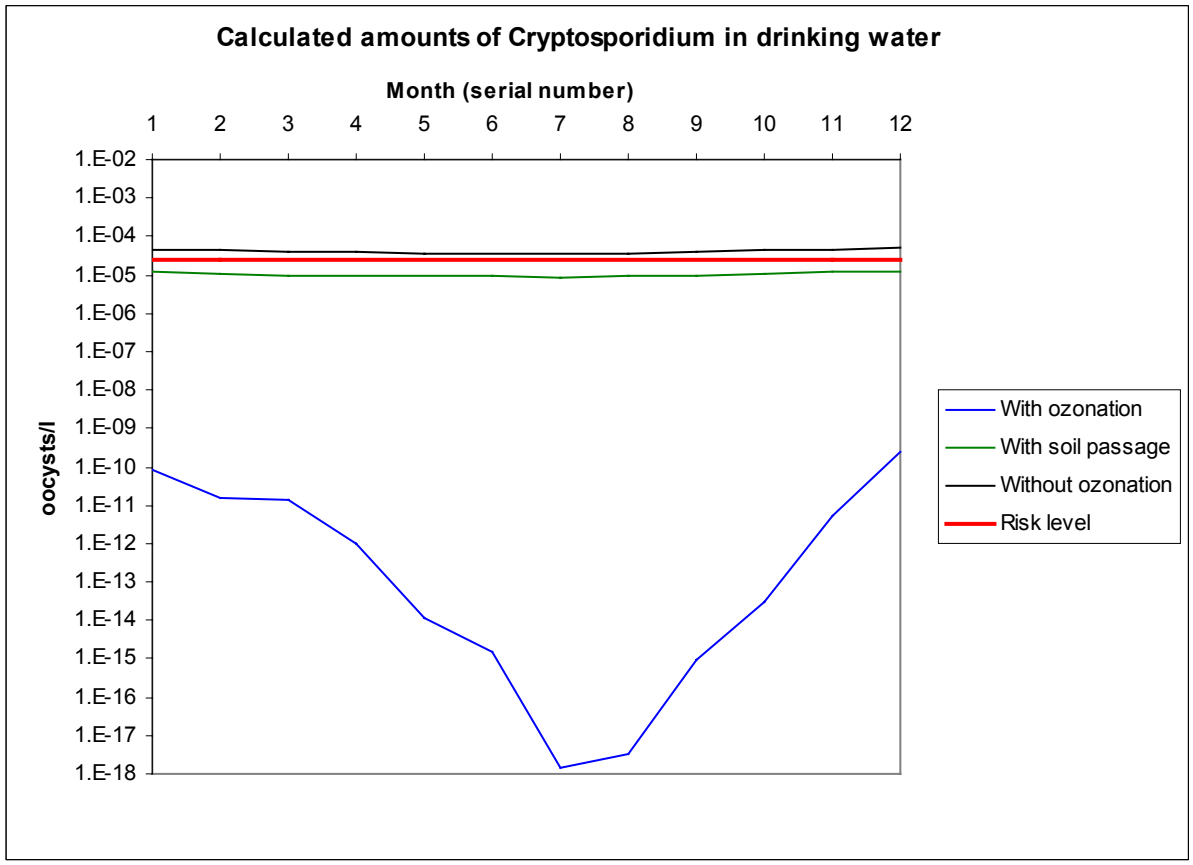

Figure 7.5 Calculated amounts of Cryptosporidium in drinking water over a year. See also 7.4.

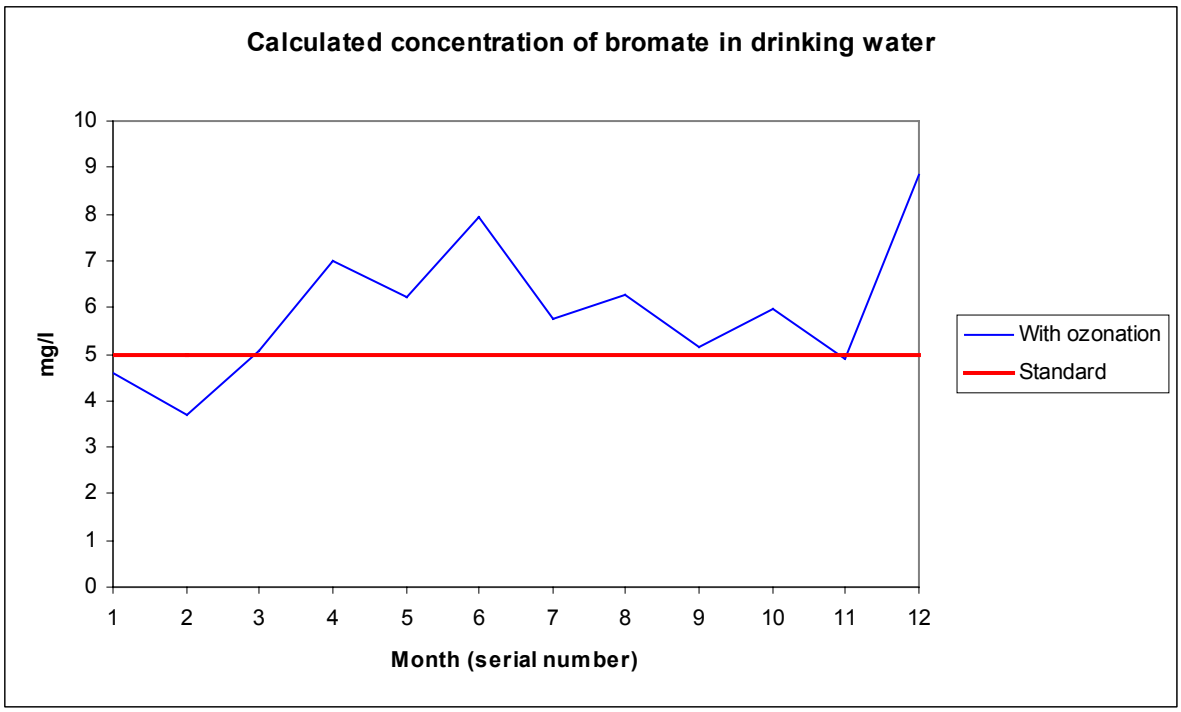

Figure 7.6 Calculated concentration of bromate in drinking water over a year

In figure 7.6 is shown the resulting concentration of bromate in the case of the treatment system with ozonation. As can be seen, this concentration is mostly above the standard of 5 µg/l (if disinfection is used), as given in the proposed Dutch Drinking-water Act (Versteegh et al .,1999). This example shows that it is possible to use TAPWAT for calculations of the quality of drinking water using a few different treatment steps. To use the model for real life calculations more calculations should be made for different treatment processes. Validation of the model is still poor, however the results donot look that bad.

7.4 Application of TAPWAT for the National Environmental Outlook

The amounts of micro-organisms present after treatment of surface water have been determined as well as the concentrations of disinfection by-products resulting form this treatment. Calculations have been made for four existing and four hypothetical treatment systems. The results are qualitatively presented in the National Environmental Outlook 1997-2020.

7.4.1 Basic assumptions

The calculations are based on future amounts of *Cryptosporidium*, *Giardia* and entero-viruses in raw water as determined with the model WATNAT, a RIVM model calculating the dispersion of substances in large Dutch surface waters. These future amounts of micro-organisms turned out to differ very little from the present state of the surface waters. Other information concerning raw surface water that was required by TAPWAT, such as pH, DOC, temperature and concentration of bromide, has therefore been based on the present quality of surface waters as available in ISDIV, the RIVM information system concerning supply of drinking and industrial water.

To determine the removal of micro-organisms, simple modules have been used consisting of a removal percentage for every treatment step. More advanced modules using ranges of removal percentages or statistical methods (see chapter 4) were not available yet at the time. The calculations concerning the formation of disinfection by-products have been performed using available process modules for ozonation and chlorination (see chapter 5).

Monte Carlo analysis hasnot been used in these calculations, owing to the fact that TAPWAT wasnot suitable for it yet. As verification of the calculated results comparisons have been made with available information concerning the quality of drinking water in ISDIV, especially the data as delivered by the drinking-water companies: the so-called REWAB-data.

7.4.2 Example of the results

As an example of the calculations that are performed, a number of results will be shown concerning the following existing Dutch treatment system:

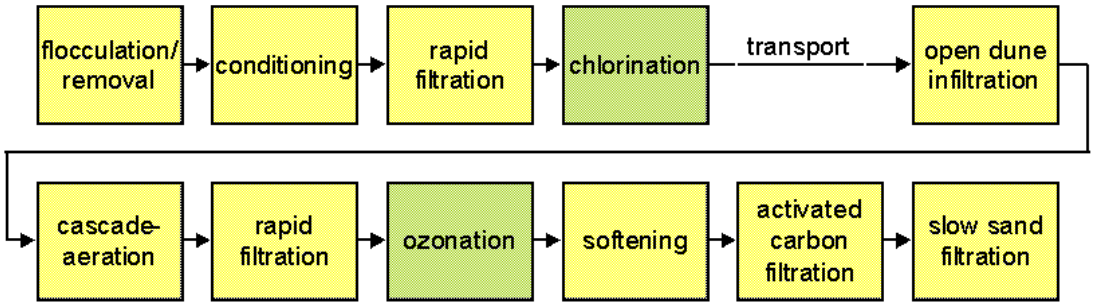

Figure 7.7 Example treatment system of the calculations for the National Outlook

The treatment steps indicated green have been represented during the calculations by process modules, the other steps by simple percentage modules.

In figure 7.8 are shown the calculated amounts of *Cryptosporidium* and *Giardia* in drinking water over the period of a year. Because of the lack of data concerning micro-organisms in drinking water, comparison with measurements is not possible.

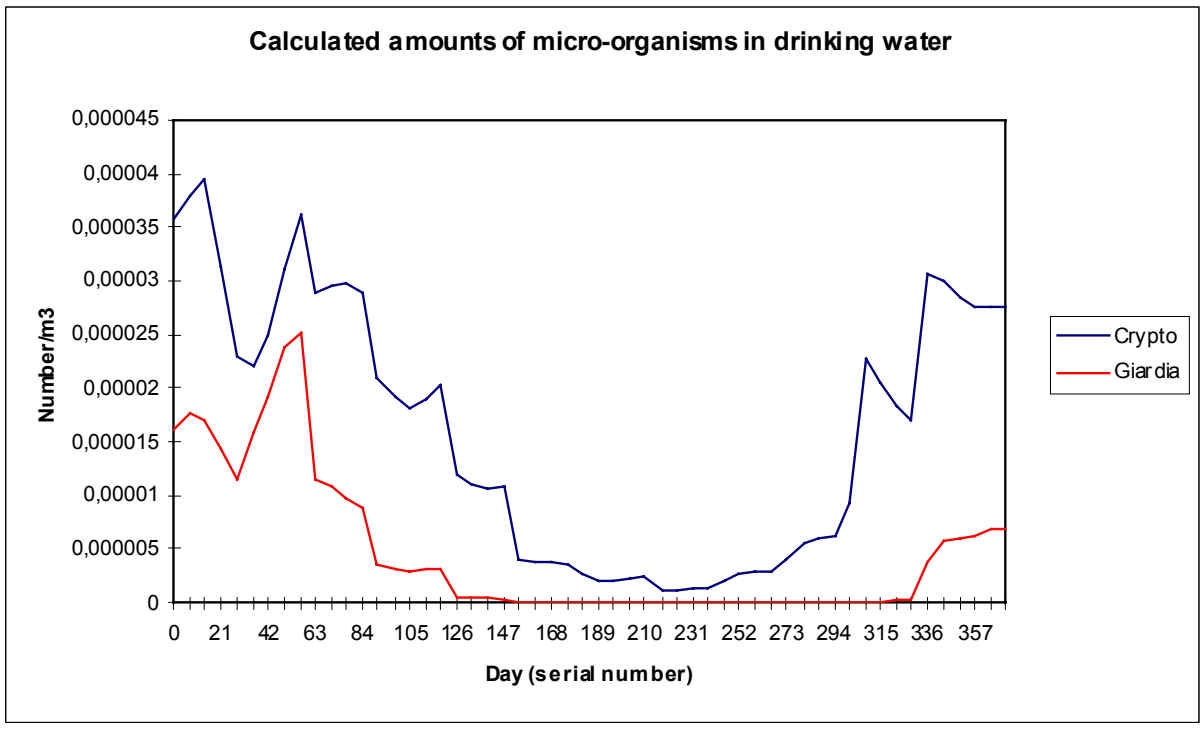

Figure 7.8 Calculated amounts of Cryptosporidium and Giardia in drinking water over the period of a year.

The resulting concentrations of disinfection by-products are shown in figure 7.9 and figure 7.10. Also shown in these graphs are the minimum, mean and maximum as measured in the treatment system in 1995.

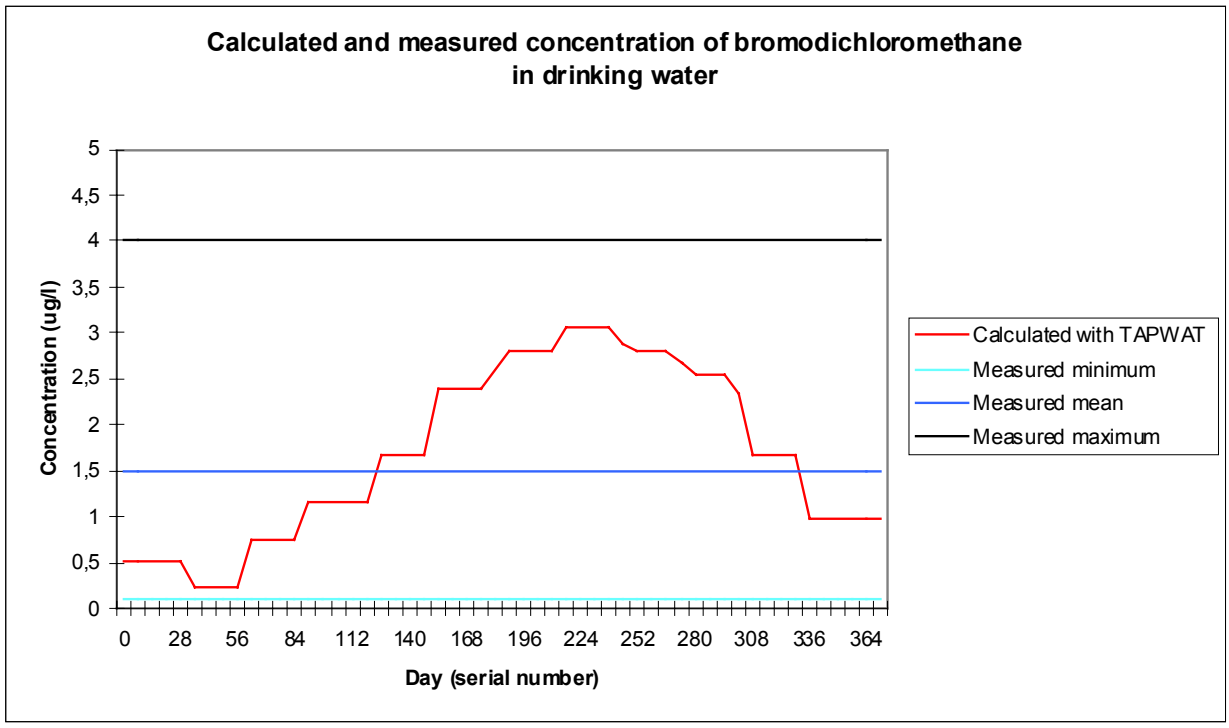

Figure 7.9 Calculated and measured concentration of bromodichloromethane in drinking water over the period of a year.

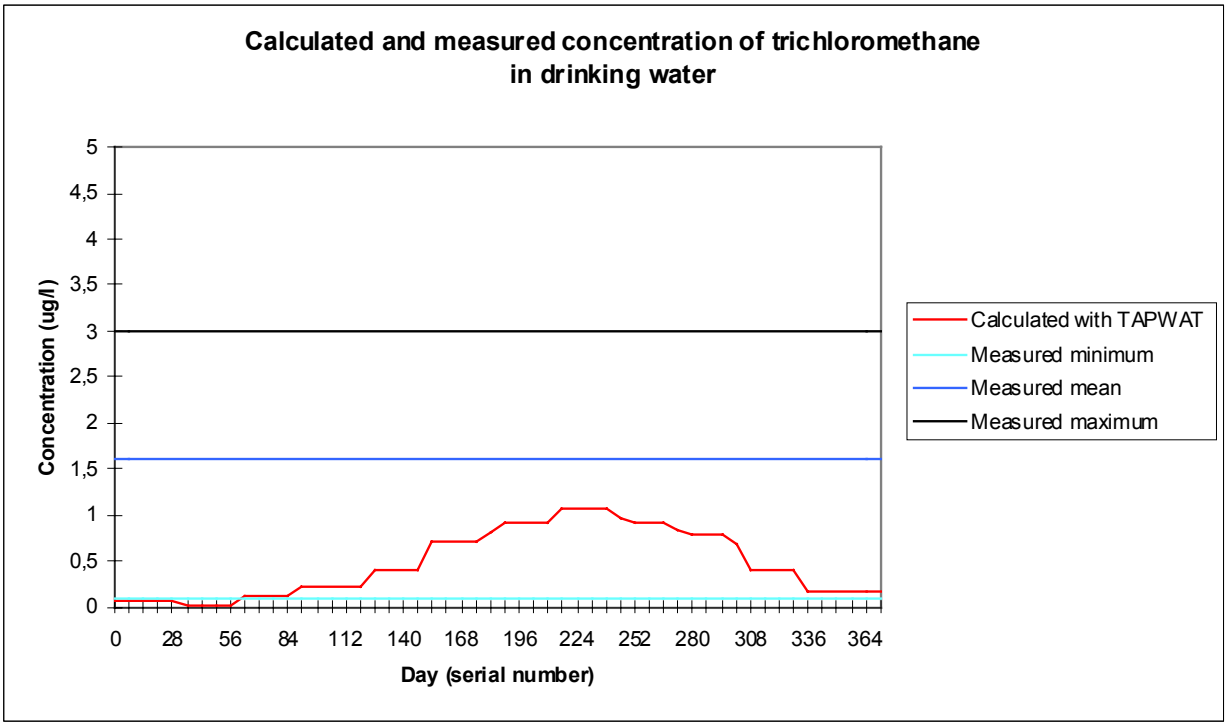

Figure 7.10 Calculated and measured concentration of trichloromethane in drinking water over the period of a year.

The results concerning disinfection by-products turn out to be reasonably consistent with the measurements of the drinking-water company concerned. Virtually all the values as calculated with TAPWAT are within the range of the minimum and maximum as measured.

7.4.3 Conclusions

On the basis of the calculations performed for this application the following can be concluded:

- The combining of percentage and process modules in calculations operates well;
- The modules used produce a workable indicative result.

However, more important is the observation that a number of aspects can be improved:

- To be able to draw better conclusions about risks for the public health, the uncertainty of the results should be considered;
- More validation is needed: comparison of calculated results with a greater number of detailed measurements from drinking-water companies.

For these reasons the results of the calculations have been entered in the text of the National Outlook in a very indicative way only; see RIVM (1997a) and RIVM (1997b).

7.5 Example of statistical analysis

In this paragraph an example of statistical analysis is presented. The beta-distribution is built into the modules floc formation and removal and active carbon filtration (GAC) (see chapter 6 for statistical analysis). Based on DOC input the daily output of DOC is calculated. The graph shows that the output has the same shape as the input. It can be concluded that the removal of DOC can be described by the beta-distribution. A disadvantage of this type of modelling is that a lot of data are needed for one parameter, which data are available for DOC but not for pathogenic micro-organisms and micropollutants. So an indicator parameter is needed.

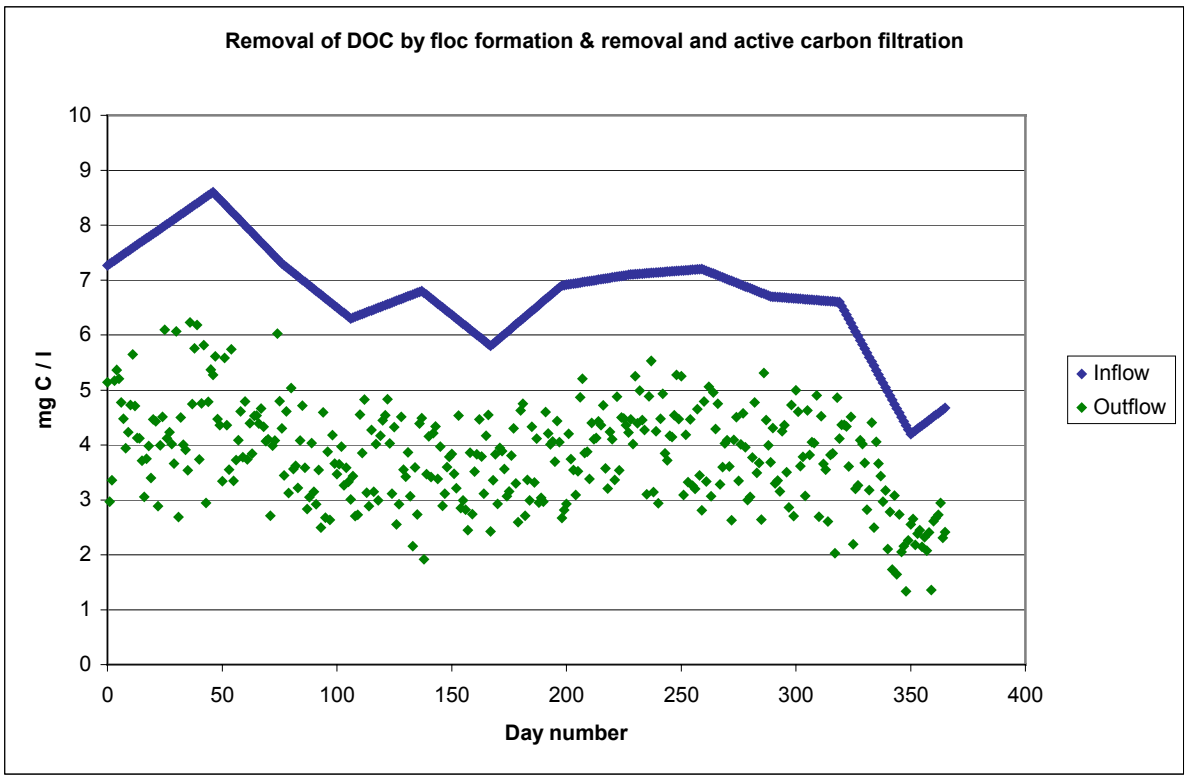

Figure 7.11 Example of a statistical module of two treatment steps based on the Beta-distribution. The graph shows a distribution of the removal of DOC calculated on a daily base.

8 Conclusions and recommendations

In this chapter conclusions and recommendations are described for the **T**ool for the **A**nalysis of the **P**roduction of drinking **WAT**er (TAPWAT).

8.1 Conclusions

The model, TAPWAT has been developed for describing drinking-water quality in integral studies. TAPWAT consists of modules that represent individual steps in a treatment process, so that different treatment processes can be constructed. The steps are used mainly in systems for the treatment of surface water. The current version of TAPWAT ,described in this report, consists of modules based on removal percentages and on process or semi-empirical modelling. In general this combination works out fairly well in the model structure developed for TAPWAT.

Modules based on removal percentages
Ranges of removal percentages are not present for all treatment steps because of limited measurement data. About 15% of the ranges are based on detailed data from water-supply companies the other are based on data from laboratory experiments and from literature. The companies don't measure a lot of individual parameters after individual treatment steps on a regularly base.
Of the data on five micro-organisms of interest for public health or an indicator, only data for spores of sulfite-reducing clostridia (SSRC) are available.
For the organic micro-pollutants and heavy metals (six compounds), data availability is very limited and even absent for two compounds.
Data availability is reasonable for disinfection by-products.

Modules based on process or semi-empirical modelling
In TAPWAT the chlorination and ozonation modules are incorporated for the prediction of disinfection by-products and the removal of micro-organisms. These modules are based on empirically based equations. Stochastic modelling is done for two treatment steps (floc formation and removal, and activated carbon filtration). Stochastic modelling using beta-distribution is a promising technique; however, the lack of available data for individual treatment steps is a disadvantage. Only indicator parameters or parameters which are easy and cheap to measure are suitable.

Model calibration and validation
The usefulness of full-scale data for model calibration is limited, because of the lack of data for individual treatment steps. These data are important; however, and should be used as much as possible for model calibration. Pilot-scale and laboratory data will have to fill the (many) gaps.
General expressions for the estimation of value μ (average in the beta-distribution) should be formulated for use in stochastic modelling. This value is specific for each treatment plant but can be made more general to improve teh usefulness of TAPWAT, for example, by analysing measurement data of more plants in the same way.
Assuming that the different parameters, influencing the removal ratio of the treatment process, are independent of each other, the beta-distribution can be used for Monte Carlo analysis of the treatment processes.

Only a few validations have been done with the model TAPWAT. For the most interesting parameters like pesticides and pathogens, either data is lacking or there are too many measurements below detection limit. Indicators should be used for the pathogens; however, there are still a lot of 'below-detection-limit' data. The subject on how to calculate the removal of micro-organisms has been described in a separate report (Evers and Groennou, 1999).
The modules in TAPWAT are based on an average performance of treatment steps; this can differ from the performance of a treatment step in a particular treatment system.
Caution will be needed when applying the model to specific cases.

8.2 Recommendations

TAPWAT is a model suitable for application on a global scale in treatment plants using surface water as the raw water source. The model described is not yet completed. The modules based on removal percentages should be updated regularly, and those based on process or semi-empirical modelling have to be validated for more systems so that uncertainty of the results can be described on a higher level.

New model studies for soil passage have been recently published (Schijven, 2001), the results of which should be incorporated in TAPWAT. Considering that UV-disinfection technique has now become more important for the removal of pathogens like viruses and protozoa, a module for UV should be incorporated in TAPWAT. Membrane technology is used more and more for piped water production like drinking water and household water. Information available from pilot and full-scale plants should be used to improve the existing modules.

The model must be able, at least for pathogens, to cover the pathway from water source to infection risk for the public. The parts of the puzzle are present but the puzzle still has to be laid.

The model is as yet only operable for experts. To make it suitable for non-experts an update of the current version with input screens etc. has to be made. This work should be put out to a contractor.

A plan of action is recommended in which the existing and missing modules, compounds and micro-organisms of interest are prioritised and the necessary validation of the model carried out. To both improve the current TAPWAT version and make it suitable for public health risk assessment the plan of action should be carried out by experts and model updates eventually put out to a contractor.

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