IMPROVING OPERATION OF DRINKING WATER TREATMENT THROUGH MODELLING

L.C. Rietveld

Propositions

belonging to the dissertation

Improving operation of drinking water treatment through modelling

Louis Cornelis Rietveld
Delft, 22 februari 2005

1. The use of phenomenological models in drinking water treatment leads to a better operation. (this dissertation)

2. An optimal operation of softening results in a better water quality as well as lower costs and less environmental impact. (this dissertation)

3. For quality reasons it is preferable to use all lanes of a treatment at all times.

4. Bubble columns for dosing ozone do not function optimally.
(Van der Helm et al., submitted to Water Research, 2004)

5. The performance of an integral operated treatment is better than that of the sum of the separately operated unit processes.
(Bosklopper et al., IWA-Conference Marrakech, 2004)

6. The quality requirements for “household water” must for operational and risk reasons be such that application is not sustainable.
(Versteegh et al., RIVM, 1997; Oesterholt, Kiwa, 2003)

7. The microbial quality of drinking water in the Netherlands is mainly determined by the level of recontamination and regrowth during treatment and distribution.
(Van der Kooij et al., J. SRT-Aqua Vol. 48 No. 1, 1999; Van Lieverloo et. al., Kiwa, 2003)

8. The introduction of a new technology requires a sound local organisation and knowledge level; this is also valid for appropriate technology in developing countries.

9. A scientist only enjoys freedom when he commits himself to a project.

10. Drinking bottled water is comparable to throwing a coin in a fountain: it gives a false sense of safety and it costs money.

These propositions are considered defendable and as such have been approved by the supervisors Prof. ir. J.C. van Dijk and Prof. dr. J. Haarhoff

Stellingen

behorende bij het proefschrift

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1 Het gebruik van fenomenologische modellen in de drinkwaterzuivering leidt tot een betere bedrijfsvoering. (dit proefschrift)

2 Een optimale bedrijfsvoering van ontharding resulteert in zowel een betere waterkwaliteit als lagere kosten en een lagere milieubelasting. (dit proefschrift)

3 Uit kwaliteitsoverwegingen is het wenselijk om alle straten van een zuivering te allen tijde in te schakelen.

4 Bellenkolommen voor de dosering van ozon werken niet optimaal.
(Van der Helm et al., submitted to Water Research, 2004)

5 De prestatie van een integraal bestuurde zuivering is beter dan die van de som van de afzonderlijk bestuurde deelprocessen.
(Bosklopper et al., IWA-Conference Marrakech, 2004)

6 De kwaliteitseisen van “huishoudwater” moeten uit bedrijfstechnische en risico-overwegingen dusdanig zijn dat het toepassen ervan niet duurzaam is.
(Versteegh et al., RIVM, 1997; Oesterholt, Kiwa, 2003)

7 De microbiologische kwaliteit van het drinkwater wordt in Nederland vooral bepaald door de mate van herbesmetting en nagroei tijdens de zuivering en distributie. (Van der Kooij et al., J. SRT-Aqua Vol. 48 No. 1, 1999; Van Lieverloo et. al., Kiwa, 2003)

8 Het introduceren van een nieuwe technologie vergt een gedegen organisatie en kennisniveau ter plaatse; dit geldt ook voor aangepaste technologie in ontwikkelingslanden.

9 Een wetenschapper geniet pas vrijheid als hij zich (ver)bindt aan een project.

10 Het drinken van flessenwater is vergelijkbaar met het gooien van een munt in een fontein: het geeft een vals gevoel van veiligheid en het kost geld.

Deze stellingen zijn verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotoren Prof. ir. J.C. van Dijk en Prof. dr. J. Haarhoff

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PROEFSCHRIFT

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus Prof. dr. ir. J.T. Fokkema,
voorzitter van het College van Promoties,
in het openbaar te verdedigen op dinsdag 22 februari 2005 om 13.00 uur
door Louis Cornelis RIETVELD
civiel ingenieur
geboren te Sint Pancras

Dit proefschrift is goedgekeurd door de promotoren:
Prof. ir. J.C. van Dijk
Prof. dr. J. Haarhoff

Samenstelling promotiecommissie:

Rector Magnificus, voorzitter
Prof. ir. J.C. van Dijk, Technische Universiteit Delft, promotor
Prof. dr. J. Haarhoff, Rand Afrikaanse Universiteit, promotor
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Prof. dr. ir. W.G.J. van der Meer, Universiteit Twente

Gutta cavat lapidem, non vi, sed saepe cadendo

CONTENTS

1 INTRODUCTION

1.1 Background of the thesis

1.1.1 Actual operation of drinking water treatment plants

To guarantee a high drinking water quality, intensive quality monitoring of the source and the product of drinking water treatment plants is performed. The product of the drinking water treatment plant has to comply with international water quality guidelines and national standards. Sometimes water companies even set more stringent guidelines for operational purposes. The water quality guidelines and standards are maximum (in some cases minimum) levels. The lower the level of the parameters is the better the water quality, but the higher the treatment costs. In addition, raw water quality is subject to changes. These can be seasonal effects (temperature, turbidity) or long-term trends (salt content). Actual raw water quality and flow can be different from what the drinking water treatment plant was designed for and it is the task of the operators to cope with the changing circumstances, complying with the water quality guidelines and standards. In general, projections are made for future demand and extra safety factors are introduced during the design, leading to an effluent water quality that is better than the levels set in the guidelines and standards.

Operation of drinking water treatment plants is nowadays based on experience. Water quality is monitored to prove that guidelines are met and, sometimes, laboratory tests are performed to determine e.g. the dosage of chemicals. All these data, however, are scarcely used to improve day-to-day operation and disappear in the cellars of the water company. Normally, operation does not include time varying aspects, but is rather fixed. With the development of on-line monitoring, more and more data are collected and stored. The problem, however, is how to obtain information from these data as input for operation.

1.1.2 Improvement of operation

To improve operation a common theme is the search for an optimal, or best, solution that is changing in time (Hillier and Lieberman, 1995). Therefore, it is necessary to come to terms with the complexity of interpreting the interactions of many contemporaneously measured parameters (Beck and Lin, 2003).

In drinking water treatment, criteria for evaluation of the operation of the processes are the following:

- Product water quality
- Operational costs
- Environmental impact
    - Energy consumption
    - Water spills in treatment and distribution
    - Use of chemical products
    - Production of sludge and waste material

A good water quality will result in the absence of public health hazards, corrosion of piping material and re-growth in the distribution network. The impact on public health is quantified using special methods based on risk assessment for determining the required water quality. In general, the microbiological guidelines are based on the assumption that an infection of 1:10000 per year is acceptable. For the micro-pollutants an upper bound excess lifetime risk of 10^{-6} (or one additional cancer per 1000,000 of the population ingesting drinking water containing the substance at the guideline value for 70 years) is accepted.

There is normally a tension between the product water quality parameters, the operational costs and the environmental impact. The more frequent the backwashing and/or regeneration of a filter, the better the product water quality, the higher the operational costs and the greater the environmental impact. It depends on local circumstances and the treatment process under consideration which criterion is predominant.

In civil engineering two basic methods are used to compare criteria of different dimensions:

- Multi-criteria analysis
- Cost evaluation

The first method is based on credits for selected criteria. The sum of the credits is an indication for the performance of the alternative under consideration. The higher the sum the better the alternative is. As not all criteria have the same impact, weighing factors are introduced in this method. In the second method all criteria are expressed in costs. In water treatment this means that product water quality has to be expressed in monetary values. One way of doing this is by expressing the risk of illness and death in terms of costs of hospitalisation and loss of productivity. The amount of money that is involved in the loss of productivity is a political consideration. The translation of environmental impact into costs is also controversial, but is easier to perform than for the product water quality. The alternative with the lowest total costs is considered to be the best.

The optimisation process is to find the maximum (in case of the multi-criteria analysis) or the minimum (in case of cost evaluation) of an objective function. This can be done by using solver functions. For a certain initial setting the value of the objective function is calculated. During the optimisation the settings are gradually changed and the values of the objective function are compared to the initial value. With an intelligent solver the surface of the values of the objective function is scanned and the maximum or minimum is found. There are several constraints on the optimisation problems. The most important constraint is that the legal obligations must be met. In drinking water treatment, this is mainly related to product water quality. In addition, there are some physical constraints. The plant cannot be operated outside the range of design.

In the Netherlands examples of control optimisation in drinking water industry have so far mainly focused on flow control. Energy consumption is lower and treatment performance is better when the produced flow is constant. This is achieved by demand prediction with empirical models and optimal use of storage facilities (Bakker et al., 2003).

1.1.3 Next generation scenario for operation

The improvement of operation of drinking water treatment will be supported by the recent developments in Information Communication Technology (ICT). By using modelling in combination with on-line monitoring and real-time control, the operation can be improved, resulting in a better and more stable water quality, better use of the installed infrastructure, lower treatment costs and/or reduction of environmental emissions. In addition, with ICT operation will be more objective and it will alleviate the problems of variable and even contradictory heuristics between different operating personnel leading to inconsistent operation, incorrect diagnosis of problems and the loss of unrecorded operating heuristics built up over years by the older generation (Olsson et al., 2003).

In February 2000 the Journal of the American Water Works Association published a “next generation scenario” for water utilities. According to the articles of Rosen (2000) and Trussel (2000), in 2050 a drinking water treatment plant will be controlled from a central control centre. Dedicated integral control programs in which advanced process and control models are incorporated will control the process. The process will be monitored on on-line qualitative and quantitative indicators. Innovative analysis techniques and (soft-) sensors supply the program with comprehensive information with which the necessary control decisions can be made and implemented. Real-time performance indicators will constantly evaluate the effectiveness of each process. Furthermore, the system can evaluate the effects of control decisions for future decision-making processes, leading to an increase in knowledge about the treatment plant. Operators will be trained to deal with calamities by flight simulator-like programs that represent a virtual treatment plant. Process information will be available on-line, both for process engineers and for managers of the company.

It is in the interest of the drinking water sector to aim for a technological breakthrough in the development of intelligent treatment processes in order to realise a significant shortening of the development time towards the projected 2050 scenario.

1.1.4 The use of Internet in operation

Using web technology all collected data from the drinking water treatment plant are available for everyone in the organisation, from the operator to the managing director. Dutch drinking water companies already use web technology for accessing water quantity data (Bakker et al., 2003). Additional advantages of the use of Internet technology are the possibilities for phased implementation, the large flexibility, the disappearance of the divisions between offices and treatment plants, and cost savings in ICT infrastructure by using the same communication structure at the offices as at the plants.

Internet technologies can provide web clients with a platform for remote monitoring of the behaviour of the process plants, as well as for remotely controlling the plants (Yang et al., 2003). With web based applications, the data can be given via PLC and SCADA to the computer and vice versa (see figure 1.1). Web based applications will play a vital role in future operation of drinking water treatment plants. The available data at the drinking water treatment plant can be stored on a local data server that can be approached via the web. From this server, data can be retrieved by operators when they are at other locations, by drinking water technologists at the office to analyse specific problems, and by the management for weekly, monthly and yearly reports.

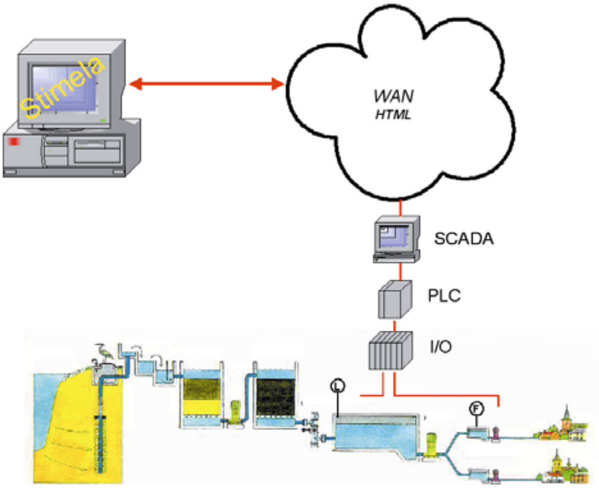

Figure 1.1 Use of Internet technology in drinking water treatment

1.1.5 The role of models in improvement of operation

The expectations of the water industry are clear: the breakthroughs are going to come in the field of automation and control (Haarhoff, 2000). Models will play a vital role in this respect and will be the interface between data and operation of drinking water treatment. The models are a reflection of the knowledge of the system and are fed by data and (new) hypotheses. Different actors in different circumstances gain knowledge about drinking water treatment processes. Operators get information from the full-scale plant, designers obtain their data from pilot plants and researchers experiment on laboratory scale. If process knowledge can be encapsulated, then it will be retained. In addition, the computer will assist decision-making in plant operation.

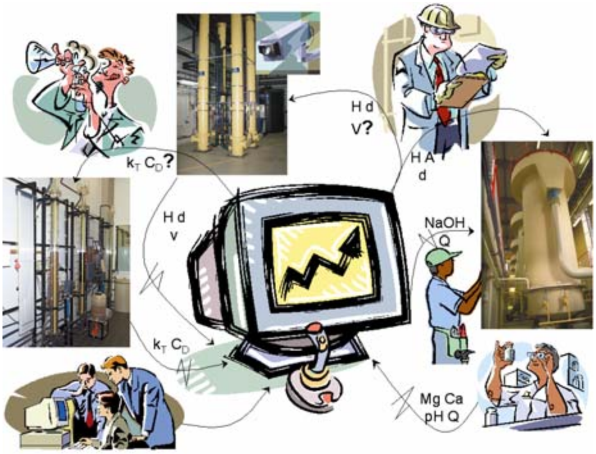

Figure 1.2 Model as a tool for exchange of knowledge

The model becomes a central point in knowledge exchange and input for calibration and validation comes from practice. Practical experiences that cannot be described by the model give input to research. Fundamental research focuses on the understanding of the processes. As a consequence, the model can assist in better understanding of the processes and more efficient pilot plant tests can be executed, resulting in an adequate design for full-scale applications (figure 1.2).

Therefore, it will be necessary to develop models to simulate the drinking water treatment processes for prediction of the behaviour of processes under changing conditions (raw water quality, flow). The simulation will lead to a virtual drinking water treatment plant that communicates with technologists, operators and managers and that can also be used for educational and training purposes.

At Delft University of Technology there is a tradition to use modelling tools in drinking water treatment. Prof.L. Huisman and Prof. H.J. Pöpel worked with static models to explain to students the mechanisms of the different treatment processes. Later, in the early nineties Prof. J.C. van Dijk used models for design optimisation (Van Dijk and Wilms, 1991, Schers and Van Dijk, 1992). All types of modelling environments were used: from a pocket calculator to Fortran codes. In the mean time it was felt that modelling would not only be important for (static) design optimisation, but in analogy to waste water treatment (Van der Kuij et al., 1994, Van Veldhuizen et al., 1999, Hulsbeek et al, 2002), the process operation could be an important field where modelling could be applied.

1.2 Objective of the thesis

The objective of the research is to demonstrate that the operation of dinking water treatment facilities can be improved through modelling. Continuous model evaluation of different operational scenarios will lead to improved operation that varies in time. Therefore, phenomenological models are used that are based on numerical integration of partial differential equations, describing the process and dynamic behaviour of the processes. The models are elaborated within the modelling environment Stimela, which is programmed in Matlab/Simulink™.

To illustrate the value of modelling for operational improvement, three cases are elaborated. The cases describe post-conventional processes, developed in the eighties, that are used in the Netherlands for polishing the drinking water after conventional treatment (floc formation, floc removal and filtration). The main polishing issues that are addressed are the removal of organic micro-pollutants, avoiding the formation of disinfection by-products, enhanced disinfection, hardness reduction and pH control. Several surface water treatment plants in the Netherlands are therefore equipped with ozonation, granular activated carbon filtration (GAC) and pellet softening and these processes are described in the cases.

1.3 Contents of the thesis

In chapter 2, a review is presented of modelling of drinking water treatment processes. Basic equations are given for transport of compounds through a reactor, transfer to a gas or solid phase, decay of the compound and mass balance between the water and the gas or solid phase. Some examples on the elaboration of these equations for conventional processes are given (aeration and gas transfer, floc formation and removal, rapid sand filtration).

In chapter 3 the processes, parameters and the requirements for a modelling environment are defined, a review of existing modelling environments is given and a description is presented of the Stimela environment, developed within the scope of the thesis. The input of the models is water flow, water quality, and manipulation and process parameters. The output consists of water quality parameters of the product of the process and some other data that describe the state of the process. The model becomes more universally applicable when numerous cases are calibrated and calibration results are stored and used in similar circumstances. Therefore, the model should be widely distributed and experiences reported. Via the website www.stimela.com modelling can be executed and experiences exchanged. This is explained at the end of the chapter

Decimal elimination of pathogenic micro-organisms during ozonation is linked to the CT-value (based on ozone concentration and residence time). The CT-value is normally only determined for contact chambers and the effect of the bubble column is neglected. In chapter 4 the first case study is presented. Ozone profiles are obtained with data from counter current flow and co-current flow reactors of the pilot plant Weesperkarspel at Amsterdam Water Supply and a model is calibrated. The model is based on partial differential equations that describe the flow of water and gas through the reactor, the transfer of ozone from the gas phase to the water and the slow and rapid decay of ozone in water.

In chapter 5 the activated carbon filters of two locations (Rodenhuis and Reijerwaard) of Hydron ZH are modelled with respect to the removal of bentazon. The activated carbon filters are installed in series of two filters in a pseudo moving bed configuration. From pilot and full-scale plant data, the run time of granular activated carbon filters is calculated under changing influent water quality and is compared to existing operation practice. The model of the GAC is based on partial differential equations that describe the transport of micro-pollutants through the filter bed, the transfer of micro-pollutants from the water phase to the solid phase and accumulation of micro-pollutants in the pores of activated carbon grains. The model is fitted on data of the pilot plant and the drinking water treatment plant (WTP) at Rodenhuis and validated on data from WTP Reijerwaard, where the preloading with natural organic matter is higher. Afterwards, strategies for operation are evaluated.

In chapter 6 the softening process is modelled and evaluated for WTP Weesperkarspel of Amsterdam Water Supply. The objective of the study was to find an optimisation in operation, minimising super-saturation of calcium ions in the mixed product of the reactors. Data were collected from one pellet softening unit of the WTP. A model was developed based on partial differential equations describing the flow through the reactor, crystallisation of calcium carbonate on the pellets, growth of the pellets, transport of the pellets through the reactor, filter bed expansion as a function of flow and pellet size and hydraulic head loss over the reactor. After validation and model evaluation actual operation was evaluated and alternative operational actions were analysed.

In chapter 7 conclusions are given on the results of the case studies with respect to operational improvements and the role of models and numerical simulation tools in operation. In addition, a perspective is given on future work that focuses on the application of the developed tools in practice and the interaction between processes in a drinking water treatment train.

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2 MODELLING OF DRINKING WATER TREATMENT PROCESSES

2.1 Introduction

Water quality models attempt to simulate changes in the concentration of pollutants as they move through the environment or a reactor. Most reactions of importance in water treatment occur in more than a single phase, i.e. multiphase reactions. One example is that a gas is mixed with water to achieve the transformation of some undesired constituents. In other cases, a solid precipitate is formed, which removes the contaminant. Various types of reactors can be used to carry out multiphase reactions. Examples characteristic of water treatment problems include stirred tanks, venturi mixers, several tanks in series, packed columns, spray towers, filters, fluidised bed reactors. Normally, they operate on a continuous basis (in contrast to batch reactors) because of the large volumes of water processed.

There are some pollutants that are sufficiently inert for their concentration to be regarded as unchanging, except by physical transport phenomena like advection and dispersion. These are referred to as conservative substances and are often useful as tracers in the calibration of water quality models. Superimposed upon these mass transport mechanisms are physical, chemical and biological processes, which also cause changes in concentration. The fate of pollutants is the resultant of interactions between mass transfer and kinetic processes (James, 1993).

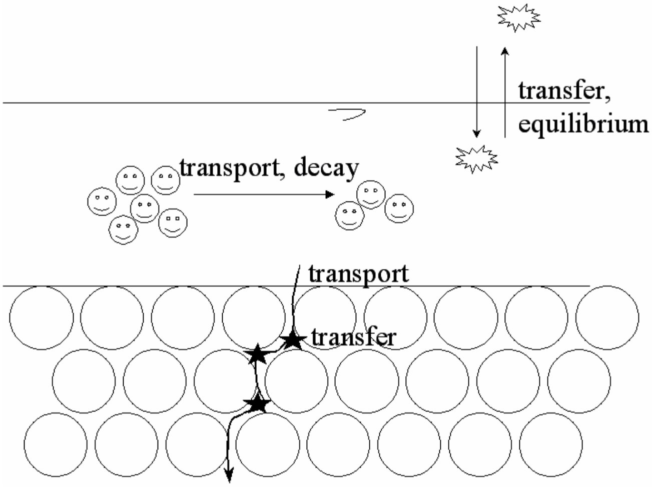

Figure 2.1 Mechanisms in treatment process

A treatment process consists of the following mechanisms (see figure 2.1):

- Flow of water containing compounds through the reactor
- Equilibrium between water and gas or solid phase
- Transfer of compounds to gas or solid phase
- Decay in the water and/or solid phase
- Mass balance between water and gas and solid phase (continuity law)

The processes in drinking water treatment have similar mechanisms and can be described with similar partial differential equations, based on the advection-dispersion model. It is the purpose of this chapter to give an overview of the basic partial differential equations for reactors in drinking water treatment. Examples are given for some of the "conventional" treatment processes for surface and groundwater:

- Aeration and gas transfer
- Floc formation and floc removal
- Rapid filtration

The description of the processes was found in literature. The contribution of the author was to write the equations in a uniform format to enable comparison of the processes and find similarities.

2.2 Basic differential equations for drinking water treatment processes

2.2.1 Transport of a compound through a reactor in water phase

Fluid behaviour in reactors is complex and difficult to describe mathematically. Two extreme, ideal flow conditions in a reactor, i.e. complete mixing and plug flow, can be distinguished. In a continuous stirred tank reactor (CSTR), the concentration of reactants and products is assumed to be uniform in all points in the reactor. In a plug flow reactor each fluid element has the same residence time. Often flow behaviour deviates substantially from the assumptions of ideal flow. There are three principal types of non-ideal fluid behaviour in processing equipment: short-circuiting and dispersion. To evaluate the effects of deviations from the ideal models the distribution of residence times must be estimated. Two (one-parameter) models are widely used in water treatment applications, the advection-dispersion model and the tank-in-series model. The advection-dispersion model draws on the analogy of diffusional mixing in plug flow reactors. The tank-in-series model assumes that the residence time distribution from any reactor can be simulated by a series of equal volume CSTR's (Montgomery, 1985).

The tank-in-series model can be used whenever the dispersion model is used and for not too large a deviation from plug flow both models give identical results, for all practical purposes (Armirtharajah et al., 1991, Levenspiel, 1999). For the description of the processes, in this chapter, the advection-dispersion model is used.

In the advection-dispersion model, there are three basic mechanisms distinguished that are responsible for the transport of dissolved and suspended solids in natural waters (James, 1993):

- Advection refers to transport due to the bulk movement of the water
- Diffusion is the transport due to migration of a solute in response to a concentration gradient as a result of Brownian motion
- Dispersion is the transport due to turbulence of the fluid and velocity shear.

The molecular diffusion can, however, generally be neglected related to the large scale mixing due to turbulence. If uncertainty exists on the flow pattern, computational fluid dynamics calculations can be performed to describe it. Schematisation towards the ideal flow schemes can subsequently be made to be incorporated in the water quality modelling.

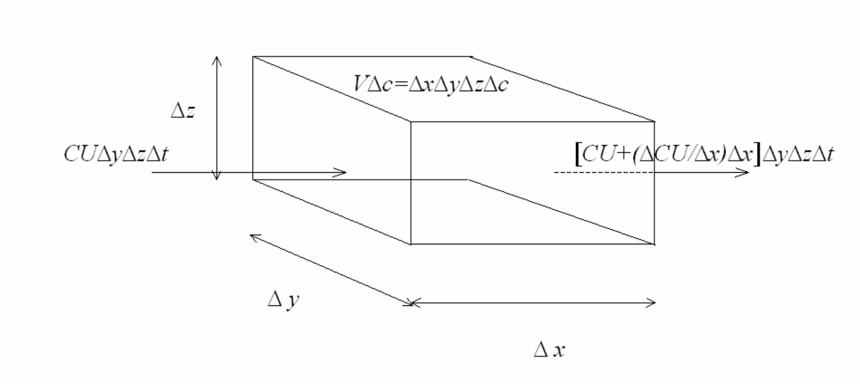

Figure 2.2 Mass balance of a conservative solute

A mass balance for a system with defined boundaries can generally be expressed as (see figure 2.2):

accumulation of mass in system = net transport into system -
net transport out of system

For a one-dimensional turbulent flow through a reactor the dissolved compounds with a concentration *C(x,y,z,t)* can be calculated with:

$$V\Delta C = \Delta x\Delta y\Delta z\Delta C = CU\Delta y\Delta z\Delta t - (CU\Delta y\Delta z\Delta t + \frac{\Delta CU}{\Delta x}\Delta x\Delta y\Delta z\Delta t)$$

$$\Rightarrow \frac{\Delta C}{\Delta t} + \frac{\Delta CU}{\Delta x} = 0$$

The instantaneous velocity component U (m/s) and concentration C (g/m^3) can be expressed as:

$$U = u + u'$$
$$C = c + c'$$

Where u and c are time-averaged components and u' and c' are turbulent components.

These expressions can be substituted into the equation, each term averaged, and with dimensions of the unit element (m) $\Delta x, \Delta y, \Delta z \rightarrow 0$ and the unit time step (s) $\Delta t \rightarrow 0$, the equation results in:

$$\frac{\partial c}{\partial t} + \frac{\partial cu}{\partial x} + \frac{\partial \overline{c'u'}}{\partial x} = 0$$

Assuming that the turbulent dispersion can be described with Fick's law for molecular diffusion, $\overline{c'u'} = -D_x \frac{dc}{dx}$, the uniform flow in x-direction, with a constant dispersion coefficient D_x (m^2/s) can be written as:

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u\frac{\partial c}{\partial x} = 0$$

2.2.2 Equilibrium of dissolved compounds between water and gas or solid phase

If water is exposed to a gas or gas mixture, a continuous exchange of gas molecules takes place from the water into the gaseous phase and vice versa. As soon as the equilibrium concentration in the water is reached both gas streams will be of equal magnitude such that no overall change of the gas concentrations in both phases occurs. This dynamic equilibrium is generally referred to as the solubility or the saturation concentration of the gas in water. The higher the gas concentration in the gaseous phase, the greater the saturation concentration in the water will be.

The relation between the saturation concentration and gas concentration in the gas phase is linear (Mueller et al., 2002):

$$c_e = K_D c_g$$

Where

c_e equilibrium concentration of compound in water (g/m^3)
c_g concentration of compound in gas phase (g/m^3)
K_D distribution coefficient (-)

In adsorption to a solid phase, saturation is determined by the adsorption capacity ($q_{\max}$ in g/kg). The adsorption capacity is determined empirically for different water concentrations. When the results are plotted on logarithmic scale a straight line is found for the relation between the water concentration and the adsorption capacity. This relation can be written by the Freundlich isotherm (Sontheimer, 1988):

$$q_{\max} = K c_e^{1/n}$$

Where

K Freundlich constant ((g/kg).(g/m^3)^n
$1/n$ Freundlich constant

If $q_{\max}$ is expressed in concentration c_s ($c_s = q_{\max}\rho_p$), the Freundlich isotherm can also be written as:

$$c_e = \left(\frac{c_s}{K\rho_p}\right)^n$$

Where

c_s concentration of compound in solid phase (g/m^3)
ρ_p particle density (kg/m^3)

If n=1 the Freundlich isotherm is linear and becomes similar to the Henry's law describing transfer of gases. Linear isotherms are typically observed for the absorption of hydrophobic substances on organic or organically coated particles (Stumm and Morgan, 1996). The general equilibrium concentration for the gas and the solid phase can thus be expressed as:

$$c_e = K_D c_{g,s}^{\ n}$$

Where

$c_{g,s}$ concentration of compound in gas or solid phase (g/m^3)
K_D distribution coefficient (g/m^3)$^{1-n}$
n constant (-)

2.2.3 Transfer of compounds to and from gas or solid phase

To count for the velocity of transfer from the water to the solid or gas phase, a kinetic equation is necessary. The rate of mass transfer of a substance across a water-solid/gas boundary has been described in terms of a diffusion film model. In general, it is necessary to consider two diffusion films, one in the water and one in the gas or solid phase. Assuming that diffusion through the water film is limiting, from Fick's first law it is concluded that the flux *F* through the water film is given by (Stumm and Morgan, 1996, Schroeder, 1977):

$$F = -D_{Br}\frac{\partial c}{\partial x}$$

The transfer by diffusion from the bulk water to the interface will thus be:

$$\frac{\partial c}{\partial t} = \frac{FA_I}{V} = -\frac{D_{Br}A}{V}\frac{\partial c}{\partial x}$$

Where

A_I interfacial area (m^2)

V volume of water (m^3)

D_{Br} diffusion coefficient (m^2/s)

F flux ($g/m^2.s$)

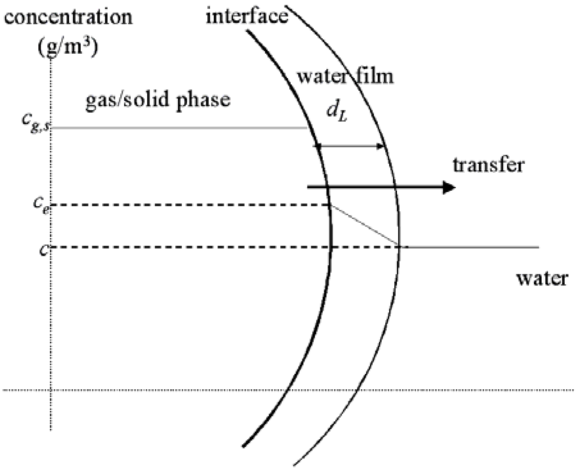

Figure 2.3 Schematic representation of one-film transfer

Through a gross simplification, linear concentration profiles are used in the water film with a sharp discontinuity between the film and the bulk phase concentration gradient, where the water concentration in the bulk water is uniform (due to turbulence). The water film coefficient is given as a function of a characteristic water film thickness d_L, resulting in (Mueller et al., 2002):

$$\frac{dc}{dt} = -D_{Br}\frac{A_I}{V}\frac{(c_e - c)}{d_L} = -k_L a(c_e - c) = -k_2(c_e - c) = f_2(c, c_{g,s})$$

Where

k_L	transfer coefficient (m/s)
a	specific surface area (m^{-1})
k_2	overall transfer coefficient (s^1)
d_L	thickness of water film (m)
f_2	transfer function

2.2.4 Reactions of compounds in water

Reaction kinetics describe the rates at which molecules are transferred into new compounds. The rate of transformation of any i^{th} reactant or product is defined as the quantity of material changing per unit time per unit volume, given as:

$$\frac{dc_i}{dt} = -f_{1,i}$$

Where

$f_{1,i}$	decay function of i^{th} reactant ($g/m^3.s$)

Simple reactions can be described by an expression for f_i. Complex reactions consist of numerous reaction paths and require multiple reaction rate expressions to describe the overall reaction rate. Finally, reactions that proceed in one direction are designated irreversible. Reactions occurring in both forward and reverse directions are known as reversible.
Often, irreversible homogeneous reactions with unknown mechanisms can be modelled with an γ-order rate expression:

$$\frac{dc_i}{dt} = -f_{1,i} = -k_1 c_i^{\gamma}$$

(Montgomery, 1985).

Where

k_1	reaction rate ($(g/m^3)^{1-\gamma}.s^{-1}$)
γ	order of reaction (-)

Assuming a first order decay, the equation can be written as:

$$\frac{dc_i}{dt} + k_1 c_i = 0$$

Resulting in the following analytical solution: $c_i = c_{i0} e^{-k_1 t}$, where k_1 is the decay rate (s^{-1}) and c_{i0} is the initial concentration (g/m^3).

2.2.5 Overall equation for fate of compound in water

The dissolved or suspended compound in water is subject to transport, transfer and degradation, the overall equation for a one-dimensional flow is therefore:

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_{g,s}) = 0$$

Where

u	velocity of water through reactor (m/s)
c	concentration of compound in water (g/m^3)
D_x	dispersion coefficient in water (m^2/s)
f_1	decay function in water
f_2	transfer function of compound from water

The first term on the left side is the change of concentration in time. When $\frac{dc}{dt} = 0$, there is a stationary situation and the concentration on a certain location is independent of time. The second term is the turbulent dispersion of the gradient type (following Fick's law). The third term indicates the transport of the concentration through the reactor by advection. The fourth term indicates a function for the decay of the compound. The last term indicates a function for the transfer of the compound from the water to the solid or gas phase.

2.2.6 Mass balance between water and gas or solid phase

The gas or solid phase can be fixed in the reactor, but can also be transported through the reactor. Flow of gas normally occurs in aerators. Flow of the solid phase can be observed in continuous sand filters or fluidised bed reactors.

The equation for this transport is:

$$\frac{\partial c_{g,s}}{\partial t} - D_{x,g,s}\frac{\partial^2 c_{g,s}}{\partial x^2} + u_{g,s}\frac{\partial c_{g,s}}{\partial x} + f_{1,g,s}(c_{g,s}) - f_{2,g,s}(c, c_{g,s}) = 0$$

Where

$u_{g,s}$	velocity of gas or solid phase through reactor (m/s)
$c_{g,s}$	concentration of compound in gas or solid phase (g/m^3)
$D_{x,g,s}$	dispersion coefficient in gas or solid phase (m^2/s)
$f_{1,g,s}$	decay function in gas or solid phase
$f_{2,g,s}$	transfer function of compound into gas or solid phase

The equation is similar to the equation of transport in water. The decay function (fourth term) is normally only present in the solid phase. For example, the concentration of the compound can be changed by (bio)-degradation. The last term indicates the function for transfer from the water to the solid or gas phase. The sign is opposite to the sign in water. The compounds that are taken from the water are stored in the solid or gas phase and vice versa.

The mass balance between the water phase and solid or gas phase can be expressed as follows (see figure 2.4):

$$\begin{aligned}
&V\Delta C + V_{g,s}\Delta C_{g,s} = \Delta x\Delta y\Delta z\Delta C + \Delta x\Delta y\Delta z_{g,s}\Delta C_{g,s} = \\
&CU\Delta y\Delta z\Delta t - (CU\Delta y\Delta z\Delta t + \frac{\Delta CU}{\Delta x}\Delta x\Delta y\Delta z\Delta t) + \ldots \\
&C_{g,s}U_{g,s}\Delta y\Delta z_{g,s}\Delta t - (C_{g,s}U_{g,s}\Delta y\Delta z_{g,s}\Delta t + \frac{\Delta C_{g,s}U_{g,s}}{\Delta x}\Delta x\Delta y\Delta z_{g,s}\Delta t)
\end{aligned}$$

with Δx, Δy, Δz, $\Delta z_{g,s}$, $\Delta t \rightarrow 0$

$$\Rightarrow V\frac{\partial C}{\partial t} + \frac{\partial CU}{\partial x}dxdydz + V_{g,s}\frac{\partial C_{g,s}}{\partial t} + \frac{\partial C_{g,s}U_{g,s}}{\partial x}dxdydz_{g,s} = 0$$

In case dispersion is neglected ($C=c$, $C_{g,s}=c_{g,s}$, $U=u$ and $U_{g,s}=u_{g,s}$), the equation can also be written as:

$$\frac{\partial c}{\partial t} + \frac{\partial cu}{\partial x} = -\frac{V_{g,s}}{V}(\frac{\partial c_{g,s}}{\partial t} + \frac{\partial c_{g,s}u_{g,s}}{\partial x})$$

Where

V	volume of water (m^3)
$V_{g,s}$	volume of gas or solid (m^3)

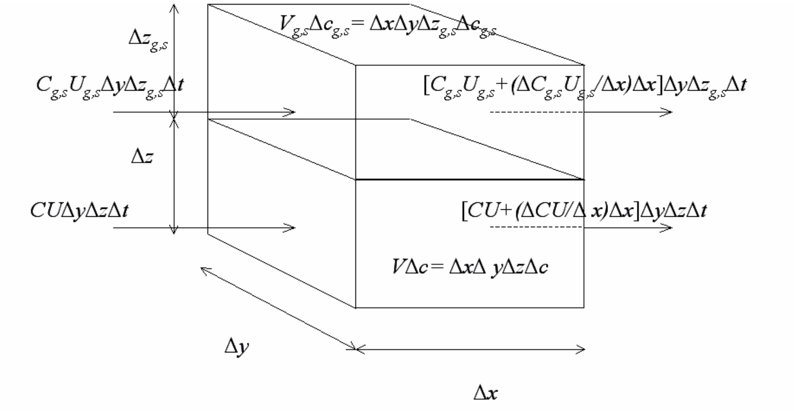

Figure 2.4 Mass balance between water and solid or gas phase

2.3 Aeration and gas transfer

Aeration is applied in drinking water treatment to exchange gasses between water and air. In case of anaerobic (ground)water, oxygen is inserted and carbon dioxide, methane and/or other volatile gases are stripped. There are several types of aerators: spray aerators, bubble aerators, cascades, tower aerators and plate aerators (Mueller et al., 2002).

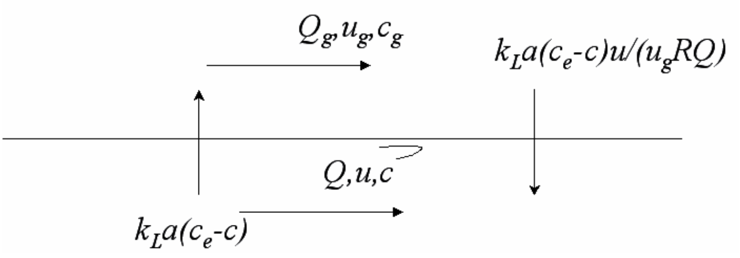

Figure 2.5 Schematic impression of co-current aeration

In case of stationary water and gas flows in an aerator, where dispersion and decay are neglected, the overall equations for transport in the water and the gas phase

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_g) = 0$$

$$\frac{\partial c_g}{\partial t} - D_{x,g} \frac{\partial^2 c_g}{\partial x^2} + u_g \frac{\partial c_g}{\partial x} + f_{1,g}(c_g) + f_{2,g}(c, c_g) = 0$$

are reduced to:

$$u\frac{dc}{dx}+f_2(c,c_g)=0$$

$$u_g\frac{dc_g}{dx}+f_{2,g}(c,c_g)=0$$

Where

$$f_2(c,c_{g,s})=k_La(K_Dc_g-c)$$

The mass balance between the water and gas phase can be written as:

$$Q_g\frac{dc_g}{dx}=-Q\frac{dc}{dx}\Rightarrow\frac{dc_g}{dx}=-\frac{Q}{Q_g}\frac{dc}{dx}=-\frac{1}{RQ}\frac{dc}{dx}$$

The change in gas concentration in the gas phase will result in an opposite change in gas concentration in the water.

Inserting this relation into the equation for gas transport in the water and the gas phase, the relation between the transfer rates from the water and from the gas phase is found:

$$\left.\begin{aligned}u\frac{dc}{dx}&=-f_2(c,c_g)\\u_g\frac{dc_g}{dx}&=f_{2,g,s}(c,c_g)\end{aligned}\right\}\Rightarrow f_{2,g}(c,c_g)=-u_g\frac{1}{RQ}\frac{\partial c}{\partial x}=\frac{u_g}{u}\frac{1}{RQ}f_2(c,c_g)$$

Where

RQ gas to water flow ratio (Q_g/Q) (Nm^3/m^3)

Q water flow (m^3/s)

Q_g gas flow (Nm^3/s)

Assuming a water and gas transport without dispersion and decay and filling in the relations of equilibrium and transfer, the equations for aeration are:

$$\frac{\partial c}{\partial t}=-u.\frac{\partial c}{\partial x}+k_L.a.(K_Dc_g-c)=-u\frac{\partial c}{\partial x}+k_2(c_e-c)$$

$$\frac{\partial c_g}{\partial t}=-u_g\frac{\partial c_g}{\partial x}-\frac{k_L.a}{RQ}\frac{u_g}{u}(K_Dc_g-c)=-u_g\frac{\partial c_g}{\partial x}-\frac{k_2}{RQ}\frac{u_g}{u}(c_e-c)$$

The saturation concentration of gas in water depends on the concentration in the gas phase and the distribution coefficient K_D. The concentration in the gas phase depends mainly on the partial pressure of the gas in the gas phase (Mueller et al., 2002; Stumm and Morgan, 1996).

For most gas-liquid problems in water treatment, resistances in the water phase control the rate of mass transfer. Typically, the k_L values range from 10^{-4} to 10^{-1} m/s in common gas-water contacting devices (Montgomery, 1985). In turbulent flow, the specific interfacial area is difficult to determine. It is common practice to measure the product of the mass transfer coefficient and the specific interfacial area, k_La or k_2.

2.4 Floc formation and floc removal

2.4.1 Floc formation

Floc formation is mainly designed as a pre-treatment step for the removal of suspended solids, turbidity and particles. During the floc formation process also heavy metals, pathogenic micro-organisms and organic matter are incorporated in the flocs. Detailed reviews of the developments in floc formation modelling can be found in literature (Bratby 1989, Armirtharajah et al., 1991). Following Haarhoff (1997), the mathematical foundations have been laid by the work of Von Smoluchowski for orhokinetic floc formation of colloidal particles under laminar flow conditions. In 1943 Camp and Stein introduced the velocity gradient G thereby extending the model to include turbulent flow regimes. The assumption was made that all particle collisions were permanent and no floc break-up was considered. Harris and Kaufmann modified the previous models to include the concepts of floc break-up. With a number of simplying assumptions Argaman-Kaufman developed an equation for floc formation in a single CSTR. By assuming that the model constants remained constant in consecutive tanks, the model was extended to and verified for a number of floc formation tanks in series.

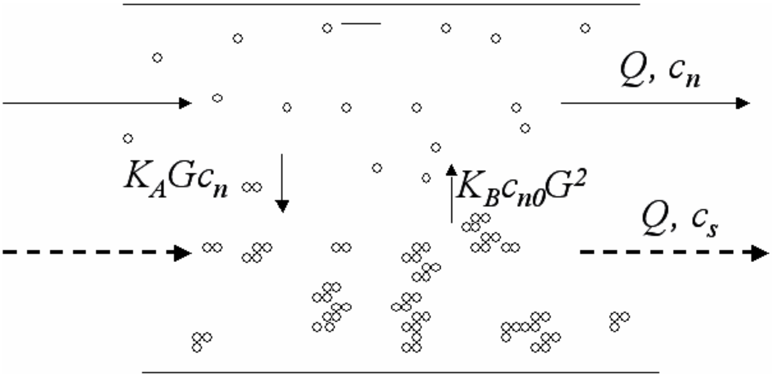

Figure 2.6 Schematic impression of floc formation chamber

The kinetics given by the Argaman-Kaufman (1970) equation for a batch CSTR can be written as:

$$\frac{dc_n}{dt} = -K_A G c_n + (K_B c_{n0}) G^2$$

Where

c_n number concentration of primary particles (m^{-3})

c_{n0} initial number concentration of primary particles (m^{-3})

K_A collision constant (-)

K_B break-up constant (s)

G velocity gradient (s^{-1})

In the Argaman-Kaufman equation it is assumed that the primary particles collide into flocs and that these flocs are removed by the subsequent particle removal device (settling, flotation, sludge blanket removal). In the absence of satisfactory means for determining the number concentration, particle mass concentration may be substituted for number concentration (Haarhoff and Joubert, 1997). In some researches, a linear relation between suspended solids concentration and turbidity is assumed and suspended solids concentration is replaced by the easy-to-measure turbidity. For the transport of suspended solids in water and in flocs, neglecting dispersion and decay, the overall equations for transport of particles in the water and solid phase

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$
$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u_s \frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}(c, c_s) = 0$$

are reduced to

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + f_2(c, c_s) = 0$$
$$\frac{\partial c_s}{\partial t} + u_s \frac{\partial c_s}{\partial x} + f_{2,s}(c, c_s) = 0$$

Where

$$f_2(c, c_s) = -f_{2,s}(c, c_s) = K_A G c - K_B c_0 G^2$$

Resulting in the following equations:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - K_A Gc + (K_B c_0)G^2 = -u\frac{\partial c}{\partial x} - K_A G(c - \frac{K_B}{K_A}Gc_0) = -u\frac{\partial c}{\partial x} - k_2(c - c_e)$$

$$\frac{\partial c_s}{\partial t} = -u\frac{\partial c_s}{\partial x} + K_A G(c - \frac{K_B}{K_A}G.c_0) = -u\frac{\partial c_s}{\partial x} + k_2(c - c_e)$$

Where:

c concentration of suspended solids as primary particles (g/m^3)

c_s concentration of suspended solids captured into flocs (g/m^3)

c_e equilibrium concentration of suspended solids captured into flocs (g/m^3)

Using the general equation then $k_2 = K_A G$ and $c_e = \frac{K_B}{K_A}Gc_0$.

Related to the general equation $c_e = K_D c_{g,s}{}^n$, this means that $K_D = \frac{K_B}{K_A}Gc_0$ and $n=0$.

From the equations it can be concluded that no floc formation will occur when G or K_A are zero and that all particles will eventually be incorporated in flocs when K_B is zero and flocs do not break-up.

The flocs are removed in subsequent separation devices: settling, flotation and filtration. The concentration of suspended solids in the flocs is the influent concentration of suspended solids in the separation devices (assuming that primary particles will not be removed in these installations).

2.4.2 Collision of flocs onto bubbles

The bubble zone during dissolved air flotation can be seen as a bubble filter where flocs can be attached to the bubbles. The collision between flocs and bubbles depends on the attachment efficiency, the size of the bubbles and the flocs, the concentration of the bubbles and the flocs, the temperature and the density.

The removal efficiency (ω) of particles by a single bubble is expressed as (Edzwald, 1995):

$$\omega = -\frac{dc}{c} = \alpha_{pb}\eta_T$$

Where

α_{pb} adhesion efficiency (-)

η_T total single collector (bubble) efficiency (-)

$$\eta_T = 0.9\left(\frac{k_B T}{\mu . d_p d_b u_b}\right)^{2/3} + \frac{3}{2}\left(\frac{d_p}{d_b}\right)^2 + (\rho_p - \rho_w) g \frac{d_p^2}{18 \mu . u_b}$$

Where

k_B	Boltzmann’s constant = 1.38 10^{-23} J/K
T	absolute temperature (K)
d_p	particle diameter (m)
ρ_p	particle density (kg/m^3)
ρ_w	water density (kg/m^3)
μ	dynamic viscosity (kg/m.s)

The first term is due to Brownian motion, the second term to fluid shear and the last term to differential sedimentation.

The following particle removal rate equation is obtained by extending the removal by a single bubble to a system containing a bubble number concentration of $c_{n,b}$ (for a stationary situation):

$$\frac{dc}{c} = -\alpha_{pb} \eta_T \frac{A_b}{A} c_{n,b} V = -\alpha_{pb} \eta_T A_b c_{n,b} \Delta x = -\alpha_{pb} \eta_T A_b c_{n,b} u_b \Delta t$$

$$=> \frac{dc}{dt} = -\alpha_{pb} \eta_T A_b c_{n,b} u_b c$$

Where

A_b	projected area of the bubble (m^2)
A_T	total surface area of the reactor (m^2)
$c_{n,b}$	bubble number concentration (m^{-3})
V_T	total volume of the reactor (m^3)
u_b	bubble rising velocity (m/s)

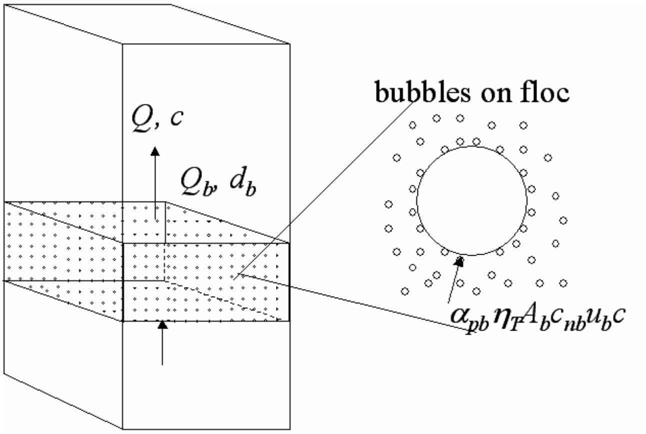

Figure 2.7 Schematic impression of flotation bubble zone

For the transport of flocs in water and on air bubbles, neglecting dispersion and decay, the overall equations for transport of flocs in the water and solid phase

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u\frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u_s \frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}(c, c_s) = 0$$

are reduced to

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} + u_s \frac{\partial c_s}{\partial x} + f_{2,s}(c, c_s) = 0$$

Where

$$f_2(c, c_s) = -f_{2,s}(c, c_s) = \alpha_{pb}\eta_T A_b c_{n,b} u_b c$$

The basic differential equation for the attachment of flocs in the bubble filter can thus be written as:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - \alpha_{pb}\eta_T A_b c_{n,b} u_b c = -u\frac{\partial c}{\partial x} - k_2 c$$

$$\frac{\partial c_s}{\partial t} = -u_s \frac{\partial c_s}{\partial x} + \alpha_{pb}\eta_T A_b c_{n,b} u_b c = -u_s \frac{\partial c_s}{\partial x} + k_2 c$$

The collision of a bubble with a floc can lead to separation of this floc in the separation zone.

The transfer coefficient k_2 is dependent on the collision and adhesion efficiency between bubbles and flocs, the number concentration of bubbles, the bubble velocity and the bubble size.

In the flotation equation the equilibrium concentration (c_e) is zero and decay of compounds in the solid phase is neglected.

2.4.3 Floc removal

Floc removal (by settling or flotation) is normally modelled by using the theory of discrete settling or flotation under ideal conditions. In settling tanks the heavy particles are separated from the water by gravity. In flotation tanks the density of the flocs, attached to air bubbles, is smaller than the density of water and the flocs will float in the separation zone.

If the size and density of the flocs is known, with a certain water temperature, the settling or flotation velocity (for laminar conditions) is given by Stokes' equation (Montgomery, 1985):

$$\mathrm{v}_s = \frac{1}{18}\frac{g}{\nu}\frac{\rho_p - \rho_w}{\rho_w} {d_p}^2$$

v_s	settling velocity of a particle (m/s)
d_p	diameter of particle (m)
$\rho_{p,w}$	density of particle and water respectively (kg/m^3)
ν	kinematic viscosity (m^2/s)

All flocs with a settling or flotation velocity $\mathrm{v}_s > Q/A$ (=surface loading) will be transferred to the sludge zone. Only part of the flocs with a settling or flotation velocity $\mathrm{v}_s < Q/A$ are removed. In practice there is a distribution of floc sizes and densities and thus a great variety of settling velocities. For a mixture of particles with different characteristics, the kinetics equation can be derived, assuming a unit element of the horizontal settling tank, neglecting decay (see figure 2.8). Here it is assumed that the removed flocs do not influence the settling rate and re-suspension is neglected.

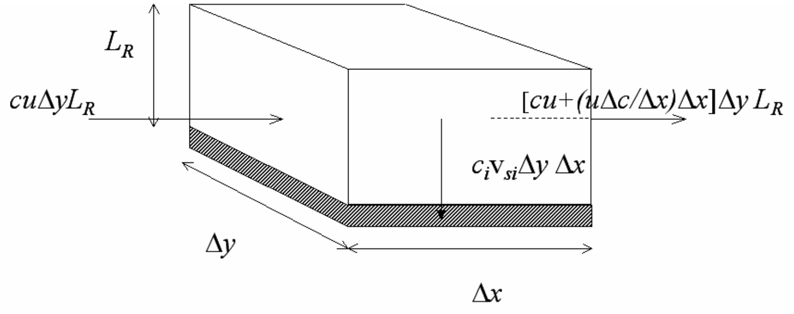

Figure 2.8 Schematic impression of horizontal settling tank

$$V\frac{\Delta c}{\Delta t} + u\frac{\Delta c}{\Delta x}\Delta x\Delta y L_R + \sum(c_i \mathrm{v}_{si}\Delta x\Delta y) = 0 \quad =>$$

$$\frac{\partial c}{\partial t} + \frac{\partial cu}{\partial x} = -\sum\left(\frac{c_i \mathrm{v}_{si}}{L_R}\right) = -\frac{\overline{\mathrm{v}_s}}{L_R}c$$

Where

$\overline{\mathrm{v}}_s$ weighted average settling velocity of particles (m/s)

L_R height of the reactor (m)

For the removal of flocs from the water phase, neglecting dispersion, decay and advection in the solid phase, the overall equations for transport of flocs

$$\frac{\partial c}{\partial t} - D_x\frac{\partial^2 c}{\partial x^2} + u\frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} - D_{x,s}\frac{\partial^2 c_s}{\partial x^2} + u_s\frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}(c, c_s) = 0$$

are reduced to

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} + f_{2,s}(c, c_s) = 0$$

Where

$$f_2(c, c_s) = -f_{2,s}(c, c_s) = \frac{\overline{\mathrm{v}_s}}{L_R}c$$

The basic differential equation for the removal of flocs can thus be written as:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - \frac{\overline{v_s}}{L_R}c = -u\frac{\partial c}{\partial x} - k_2 c$$

$$\frac{\partial c_s}{\partial t} = -u_s\frac{\partial c_s}{\partial x} + \frac{\overline{v_s}}{L_R}c = -u_s\frac{\partial c_s}{\partial x} + k_2 c$$

The settling in the unit element is dependent on different concentrations of fractions *i* and the corresponding settling velocities $v_{s,i}$. The model is described by the factor k_2, which depends on the weighted average of the settling velocities of the fractions and the height of the reactor. The constant k_2 will be dependent on the raw water characteristics and the preceding floc formation step. If there is more silt in the water, the flocs will have a higher density. In addition, with higher rotation velocities in the floc formation units, the flocs will have a higher density, but smaller sizes. The sludge accumulation c_s (in g/m^3) changes over the length of the reactor.

Related to the general equation for equilibrium $c_e = K_D c_{g,s}{}^n$, in the equation for separation the equilibrium concentration (c_e) is zero, which means that $K_d = 0$.

In conclusion, for flotation three mechanisms in series exist that determine the removal of suspended solids: collision of particles into flocs, collision of flocs onto bubbles and separation of the flocs.

2.5 Rapid filtration

Rapid filtration is normally installed after floc formation, aeration and/or softening to remove the remaining particles and flocs formed during these processes. Water flows through a (sand) bed while the grains capture the particles and flocs. During the filtration process solids accumulate in the bed and the filtration efficiency is reduced until the filter is clogged (resulting in a too high resistance or inferior product quality). Then the filter is cleaned up by backwashing and the process can be started-up again.

For the removal of solids from the water phase, neglecting dispersion, decay and advection in the solid phase and considering the water velocity in the pores, the overall equations for transport of solids

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u_s \frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,g}(c, c_s) = 0$$

are reduced to:

$$\frac{\partial c}{\partial t} + \frac{u}{\varepsilon} \frac{\partial c}{\partial x} + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} + f_{2,s}(c, c_s) = 0$$

For a stationary flow, the mass balance can be written as:

$$\left.\begin{aligned} &\frac{u}{\varepsilon} \frac{\partial c}{\partial x} = -f_2(c, c_s) \\ &\frac{\partial c_s}{\partial t} = -f_{2,s}(c, c_s) = -u \frac{\partial c}{\partial x} \end{aligned}\right\} \Rightarrow f_{2,s}(c, c_s) = -\varepsilon f_2(c, c_s)$$

Where

$$f_{2,s}(c, c_s) = -\frac{u}{\varepsilon} k_2 c$$

The concentration of the compound in the solid phase is given as mass per volume reactor, whereas water flows with pore velocity u/ε (m/s). The transfer rate to the solid phase is therefore lower than the transfer rate from the water. The difference is calculated by multiplication with the porosity ε (-).

The filtration rate k_2 is dependent on the clean bed filtration coefficient λ_0 and the concentration of removed solids. Several authors have tried to determine the clean bed filtration rate λ_0 in an empirical way for different circumstances.

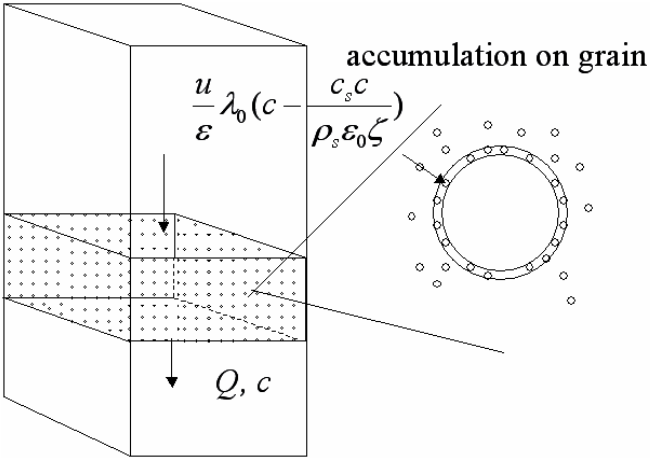

Figure 2.9 Schematic impression of rapid filter

A more scientific approach was first adapted by Yao (1971), who used the theory of floc formation of Von Smoluchowski as a basis to determine λ_0. Many of the relations between the clean bed filtration rate and the accumulated solids, can be derived from a general equation proposed by Ives (Ives, 1968, Ives, 1975, Amirharajah, 1988):

$$k_2 = \frac{u}{\varepsilon}\lambda_0(1+\frac{c_s}{1-\varepsilon_0})^{b1}(1-\frac{c_s}{\varepsilon_0})^{b2}(1-\frac{c_s}{c_{s,u}})^{b3}$$

Where

$c_{s,u}$ saturation concentration of solids in filter (g/m^3)

$b_{1,2,3}$ constants (-)

One of the simplest elaborations on this equation is given by Maroudas and Eisenklam (1965), assuming that $b_{1,2} = 0$ and $b_3 = 1$.

$$\left.\begin{aligned} k_2 &= \frac{u}{\varepsilon}\lambda_0(1-\frac{c_s}{c_{s,u}}) \\ c_{s,u} &= \varepsilon_0\rho_s\zeta \end{aligned}\right\} \Rightarrow k_2 = \frac{u}{\varepsilon}\lambda_0(1-\frac{c_s}{\varepsilon_0\rho_s\zeta})$$

Where

ζ maximum pore filling (-)

λ_0 clean bed filtration coefficient (m^{-1})

ρ_s density of solids (kg/m^3)

ε porosity (-)

ε_0 clean bed porosity (-)

In the equations the equilibrium concentration c_e is linearly dependent on the inflowing concentration.

$$c_e = \frac{c_s}{\rho_s \varepsilon_0 \zeta} c$$

The kinetics equation is then given by:

$$\frac{\partial c}{\partial t} = -\frac{u}{\varepsilon}\frac{\partial c}{\partial x} - \frac{u}{\varepsilon}\lambda_0 (c - \frac{c_s c}{\rho_s \varepsilon_0 \zeta})$$

It assumes that the effluent concentration is constantly increasing during the process (assuming a constant inflow concentration). As clogging proceeds the interstitial velocities rise from u/ε_0 to $u/(\varepsilon_0 - c_s/\rho_s)$, hindering deposition. Ultimately scour will prevent a further transfer of impurities from the water to the filter grain surfaces. At this depth c_e is equal to c, shifting the burden of removal to greater depths and augmenting the concentration of impurities in the effluent.

Comparing to the equilibrium equation $c_e = K_D {c_{g,s}}^n$, it can be concluded that for the equilibrium concentration n=1 and for the Maroudas equation $K_D = \frac{c}{\rho_s \varepsilon_0 \zeta}$.

The kinetic constant λ_0 has been studied by several researchers. Lerk proposes (Heertjes and Lerk, 1967):

$$\lambda_0 \sim \frac{1}{\nu \, \mathrm{d_p}^3}$$

Where

d_p grain diameter (m)

2.6 Discussion

In this chapter the basic principles of water quality modelling are addressed and applied to several conventional drinking water treatment processes.

The design of a reactor for the treatment of drinking water is largely dependent on the rate of transfer and reactions that take place. The higher the rate of transfer or degradation, the shorter the contact time can be to have a certain removal efficiency and the higher the velocities in a certain reactor. Velocities in reactors are in the range of 0.25 m/h (slow sand filtration) to 100 m/h (pellet softening). When the reactor is operated at high velocities, the surface area of the units can be small and the installation can thus be cheaper. In some cases, however, from a transfer point of view high velocities can be adopted, but constraints exist in rapid clogging and hydraulic resistance (membrane filtration, slow sand filtration).

The transfer rate is determined by the constant k_2 that has different values in different processes. For floc formation, separation, and filtration k_2-values are in a range of 10^{-4}-10^{-2} s^{-1}. For gas transfer the k_2-values are in a range of 10^{-1}-10^{-2} s^{-1}. This difference can also be observed in practice. The loading of gas transfer units is bigger than the loading of floc formation, separation, and filtration reactors.

The equilibrium concentration of some of the treatment processes is proportional to the accumulated concentration in the gas or solid phase (filtration and gas transfer). In this case Henry's equation is valid (n=1). If n=0, the saturation concentration is constant and determined by K_D. This also applies to floc formation where the equilibrium concentration is independent of the accumulated concentration in the solids phase, but determined by floc characteristics and G-value. When $K_D = 0$, the equilibrium concentration is equal to zero, which means that transfer is independent of the transferred substances. The equilibrium concentrations of the flotation and separation processes are zero. Therefore, under the prevailing assumptions, the processes are not inhibited by the external factors.

For a completely mixed unit element of an aeration system, the removal efficiency (ω) can be calculated with:

$$\omega = \frac{c_{i-1} - c_i}{c_{ei-1} - c_i} = \frac{1}{1 + \frac{1}{k_2 \Delta t} + \frac{K_D}{RQ}}$$

This means that with large $k_2\Delta t$ and RQ values and with a small value for K_D, the efficiency is high and vice versa. If $K_D/RQ > (k_2\Delta t)^{-1}$ the system is limited by the dissolving characteristics of the compound. If $k_2\Delta t < RQ/K_D$ the system is limited by kinetics.

Some of the other conventional drinking water treatment processes can be analysed in the same way. In case of floc removal and flotation the equilibrium concentration is neglected and the efficiency is determined by the kinetics. During floc formation, equilibrium exists between the primary particles and the flocs. Floc break-up results in the formation of primary particles, whereas collision results in the formation of flocs. If the floc break-up constant (K_B) is small compared to the collision constant (K_A), the process is dominated by kinetics.

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3 MODELLING WITHIN THE STIMELA ENVIRONMENT

3.1 Introduction

The differential equations described in the preceding chapter form the basis of phenomenological models that simulate the performance of individual treatment processes. By integrating the differential equations numerically the dynamic behaviour of the processes can be followed.

For the purpose of this thesis the modelling environment Stimela was developed. In this chapter the background and the elaboration of the modelling environment are explained. First the processes and the parameters are defined. This is followed by an analysis of what the goals for modelling are and existing modelling environments are evaluated. Finally, the Stimela environment is described including Internet applications and modelling approach.

3.2 Definition of processes and parameters

A drinking water treatment model simulates the change of water quality parameters by treatment processes. For the development of a model it is therefore of importance to define which water quality parameters must be considered and what the interrelation is between the water quality parameters and the processes.

In Dutch law the following categories of drinking water quality parameters are distinguished:

- Microbiological parameters
- Chemical parameters
- Indicator parameters
    - technical parameters
    - esthetical parameters
    - signal parameters

WHO distinguishes the parameters given in figure 3.1. For technological and modelling purposes it is not the origin of the parameters but the characteristics of the parameters that are of importance. In the classification duplications should also be avoided. In this case, the WHO classification is not suitable and another one is developed (see figure 3.2).

- Microbial aspects
  - Water-borne pathogens
- Chemical parameters
  - Naturally occurring chemicals
  - Chemicals from industrial sources and human dwellings
  - Chemicals from agricultural activities
  - Chemicals used in water treatment of materials in contact with drinking water
  - Pesticides used in water for public health purposes
  - Cyanobacterial toxins
- Radiological parameters
- Acceptability
  - Taste and odour
  - Appearance
  - Temperature

Figure 3.1 Summary of water quality parameters in WHO guidelines

- Physical/organoleptical parameters
- Microbial parameters
  - Water-borne pathogens
  - Hydrobiological parameters
- Chemical parameters
  - Hardness related parameters
  - Inorganic macro-parameters
  - Inorganic micro-parameters
  - Organic macro-parameters
  - Organic micro-parameters
  - Pesticides
  - Disinfection products
  - Disinfection by-products
- Radiological parameters

Figure 3.2 Summary of proposed water quality parameters for modelling purposes

The basic difference between the two classifications is that organoleptical and physical parameters are distinguished separately and that different subdivisions of the chemical parameters are made. Most of the parameters are health related, technical or indicator parameters. For modelling it is also of importance to distinguish parameters that influence the performance of the process. Examples are: temperature, pH, Electrical Conductivity (EC), turbidity and suspended solids, bromide, phosphate, oxygen and natural organic matter (NOM). Many treatment processes function more efficiently at higher temperatures. In drinking water treatment water temperature is not changed. Nevertheless, to model the kinetics in a reactor, temperature is of importance. In some cases pH and EC influence the process. pH is mainly determined by the concentration of carbon dioxide and bicarbonate. During (bio)chemical reactions these concentrations change and pH is thus influenced. EC is dependent on salt content. During softening and membrane processes this content changes and EC decreases. With biological processes nutrients, like phosphate and oxygen, can become limiting and should therefore be considered. Bromide and NOM influence the formation of disinfection by-products during ozonation and chlorination.

In the Netherlands different treatment trains exist for the treatment of surface and groundwater. This depends on the source water, location and tradition. In table 3.1 the main processes are shown, including the most important design and operational parameters and its effect on water quality parameters. The performance of the treatment processes is mainly determined by the design parameters.

The operation of drinking water treatment processes is characterised by three types of parameters:

- Disturbance parameters
- Controlled parameters
- Manipulated parameters

The disturbance parameters influence the behaviour of a treatment plant without being able to change them. These are the influent water quality and the flow. The controlled parameters are in general the product water quality parameters. Guidelines are given for drinking water and the product of the treatment plant should meet these guidelines. The manipulated parameters influence the treatment plant by active control. The manipulated parameters can be changed when disturbance takes place in order to maintain the controlled parameter on the desired level. In a drinking water production plant a few possibilities for active control can be distinguished. Examples are: dosage of chemicals, distribution of flow over the treatment units, air dosage in flotation units, backwash procedure and intervals of filters, run time of activated carbon filters. In practice, the operational parameters are normally set as a constant (during a certain period).

Table 3.1 Overview of the drinking water treatment processes with the relevant design, operational and water quality parameters.

Treatment processes	Design parameters	Operational parameters	Water quality parameters
Storage reservoir	Residence time, depth, aeration device		Suspended solids, NH_4^+, pathogens
Soil passage - river bank filtration - infiltration	Residence time, filtration length, structure subsoil		Suspended solids, pathogens, DOC, O_2, NH_4^+, Fe^{2+}, Mn^{2+}
Microsieves	Mesh size		Suspended solids
Floc formation	Type of coagulants, type of dosing, mixing intensity, number and size of compartments	Coagulants dose, pH, mixing intensity	Suspended solids, DOC, pH, pathogens
Floc removal - settling - flotation - sludge blanket	Surface loading, flow pattern, overflow rate, inclination of plates (titled plate settling), air flow and bubble size (flotation)	Air flow (flotation), sludge removal frequency	Suspended solids, pathogens
Rapid sand filter	Filtration rate, bed height, size of media, number of layers, supernatant water height	Water distribution over filters, run time, back wash routine	Suspended solids, pathogens, O_2, NH_4^+, Fe^{2+}, Mn^{2+}
Granular activated carbon filtration	Empty bed contact time, type of carbon, run time and see rapid sand filter	Water distribution over filters, regeneration time, run time	DOC, OMP, DBP
Oxidation/ disinfection - clorine - ozone	Contact time, dosing type	Dose of oxidant/disinfectant	Pathogens, UV-extinction, O_2, NH_4^+, DBP
Slow sand filtration	Filtration rate, bed height, media size	Water distribution over filters, run time	Pathogens, AOC
Aeration - tower aerator - cascades - plate aerator - sprinklers	Size of the reactor, number of units, surface loading/ overflow rate, packing material (tower), RQ, flow direction	Water distribution over units, air to water ratio	O_2, CH_4, CO_2 (pH), H_2S, Fe^{2+}
Pellet softening	Bed height, water flow rate, chemical products, size of reactor	Dose, by-pass flow, pellet removal rate	Ca, CO_2, HCO_3^-, pH
Micro-/ultrafiltration	Flux	cleaning procedure, transmembrane pressure	Suspended solids, pathogens
Nanofiltration/Reverse Osmosis	Flux, recovery, configuration	chemical cleaning procedure, transmembrane pressure	Pathogens, DOC, OMP, inorganics

3.3 Modelling goals

Modelling for the improvement of operation, design, research and education is preferably done in the same modelling environment, to stimulate the exchange of knowledge by different users. For each purpose there are different demands with respect to the modelling environment. In the following an inventory is made.

3.3.1 Modelling for operation

Operators can use models for real-time optimisation of operation, depending on perturbations in raw water flow and quality. For operational use of models the following requirements for the modelling environment can be identified:

- Robust modelling, without making changes in source code
- Easy calibration on available (on-line) data of full-scale plant
- Adequate graphical output for comparison between calculated and measured data
- Possibility for comparison of different operational scenarios
- Evaluation of possibilities for the interaction between different processes
- Optimisation criteria for the performance of the treatment plant
- Interaction with the installed control devices
-

3.3.2 Modelling for design

Engineers/technologists can use models to evaluate pilot and full-scale plants and come to improvements in design and operation. For design purposes the following requirements for the modelling environment can be identified:

- Robust modelling, without making changes in source code
- Easy calibration on available (on-line) data of full-scale or pilot plant
- Adequate graphical output for comparison between calculated and measured data
- Possibility for comparison of different (operational and) design scenarios
- Evaluation of possibilities for the interaction between different processes
- Optimisation criteria for the performance of the treatment plant

3.3.3 Modelling for fundamental research

Fundamental research is normally focussed on one single process. In general, the existing model is not adequate to describe all the phenomena to be studied and the model must therefore be adapted. The water researcher is less interested in studying the basic software. Therefore the modelling environment must have the following requirements:

- An open structure with possibilities for adaptations
- Easy to use and program
- Standardised in set up so that it can be connected to other models and transparency is promoted
- Availability of basic modules and algorithms
- Adequate graphical output for reporting and comparisons

3.3.4 Modelling for education purposes

Treatment plants (in the Netherlands) are safe and robust and calamities do not occur. As a result, operators and engineers lack practical experience. Therefore, models can help the instruction and training of engineers, students and operators. The following requirements can be formulated:

- Visual demonstration of phenomena in the treatment process (build up of head loss in filter, floc formation and sedimentation, growth of pellets during softening, break-through of GAC filter)
- Demonstration of the consequences of operation and design on several water quality parameters (influence of dosing on floc formation process, influence of water quality parameters on CT value during ozonation, influence of grain size of filtration media on head loss build up and effluent water quality)
- Possibilities for calibration of the model with data obtained during educational laboratory tests and extrapolation of results
- Application for pre-design of treatment plants, using default values for model parameters. Occasionally this can be in combination with the laboratory tests mentioned previously
- Decision support tool for calamities and other occasions with respect to operation

3.4 Existing modelling environments for drinking water treatment

Different models exist for the evaluation of drinking water treatment processes. Apart from "home made" programs in different programming languages and well developed programs for individual treatment processes only a few packages exist for the simulation of processes of the entire treatment plant. In the following these models are discussed.

Otter

Otter, developed by WRc, UK, is a PC based modelling package designed to dynamically simulate the performance of water treatment works (Head et al., 2002). The software can be used to simulate individual treatment processes or the whole treatment plant. The model enables process scientists and plant operators to optimise the response of the works to changes in the raw water quality, plant throughput or process operating conditions. Typical uses of the software include operational decision support, works optimisation, plant design and operator training. Version 2 of Otter includes:

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

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

Metrex

Metrex is being developed at the University of Duisburg/Germany (Mälzer and Nahrstedt, 2002). The simulation tools combine analytical and numerical models of common treatment steps used in surface water treatment (microstraining, ozonation, floc formation, sedimentation, rapid filtration, granular activated carbon filtration, biodegradation, disinfection). The emphasis is put on particle removal (particle size distributions are considered) and ozonation (oxidation of dissolved organic carbon, iron and manganese, formation of bromate). Simulated plants can be configured in any combination of treatment steps. A graphical user interface assists with detailed descriptions of the underlying mathematical models for each step and reasonable data proposals. Two levels of simulation exist. Level one is designed to simulate the whole treatment process in operation mode. Level two provides support in designing and dimensioning single process steps. The software concept is based on an object oriented model using Java technology, World-Wide-Web (WWW) browsers and the simulation software tool Matlab/ Simulink™. Each process step is designed with a uniform structure. Water compounds are characterized by their concentrations and in some cases additionally by their treatability (e.g. biodegradability, adsorbability on activated carbon). Reports of the simulation results including all water parameters are generated automatically in Hyper-Text-Markup-Language (HTML) format. Expert documentation is given by structured hypertext modules. The models used for the simulation tools of the treatment steps are mechanistic ones. In many cases qualitative knowledge exists about the range of values of the parameters and their dependencies on other known variables. This enables the user to estimate values for parameters by fuzzy-linguistic modelling.

WTP Model

The Water Treatment Plant (WTP) model was originally developed by the Environmental Protection Agency, in support of the Disinfectant/Disinfection By-products (D/DBP) Rule (Harrington et al., 1992). It is based on empirical relations obtained from regression analysis. It was prepared with the understanding that the predictions should reflect the central tendency for treatment and it is focussed on the removal of NOM, the formation of DBPs and disinfection. It is not to be construed that the results from the model will necessarily be applicable to individual raw water quality and treatment effects at unique municipalities. This model does not replace sound engineering judgement based on site-specific treatability data to evaluate the best manner in which to address the requirements of the Surface Water Treatment Rule (SWTR) or potential D/DBP Rule. It is understood that one limitation of the model is the extent of the database availability to verify model predictions. In a desire to systematically improve the overall predictive capability, the intent of the model is to solicit public comment on the usefulness and relative accuracy of the predictions on a case-by-case basis. WTP model includes a method to enter laboratory analysis so that a comparison can be made to the model predictions. In 2000 WTP model was modified. Old algorithms were updated and new process algorithms were added, especially related to inactivation of micro-organisms, formation of DBPs and the decay of disinfectants.

TAPWAT

TAPWAT (Tool for the Analysis of the Production of drinking WATer) is elaborated by the Netherlands Institute of Public Health and the Environment (RIVM), with the following goals:

- To predict on a global scale, the quality of drinking water (including health 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 along two pathways: empirical or percentages and process modules. The modules are incorporated in one model structure so the modules from both pathways can be used for one application. The model is developed according to RIVM standards for information infrastructure and modelling (Versteegh et al., 2001).

The main purpose of TAPWAT is to determine the probability of occurrence of pathogenic micro-organisms and DBPs in the product of a treatment plant, consisting of different steps in series. Different modelling approaches were adopted:

- percentage removal
- process or semi-empirical modelling
- stochastic modelling

Percentage removal. Information was collected from literature, reports, data from production plants and sometimes expert judgement to design ranges of percentages for removal of micro-organisms and compounds by the selected treatment steps.
Process modelling. A few modules for the formation of DBPs by chlorination and ozonation are tested on data of full scale plants in the Netherlands.
Stochastic modelling. The beta-distribution is used for statistical analysis of data of production plants especially for the removal of TOC and turbidity by floc formation and floc removal and activated carbon filtration (Versteegh et al., 2001).

The distribution of the product water quality parameters is determined by the distribution of the influent water quality parameters and the distribution of the removal percentages. For this, Monte Carlo techniques are used.

3.5 Modelling environment Stimela, dynamic simulation of treatment processes

3.5.1 Introduction

Eacht of the water treatment plant models discussed above, has its specific characteristics. WTP model was developed to simulate the general case rather than the site-specific case. Some drinking water treatment plant operators may be tempted to use this model as a substitute for site-specific studies. However, the output from the model is not intended to, nor should it, replace sound engineering judgement based on bench-, pilot-, and field-scale treatability studies for specific waters (Harrington et al., 1992). In fact, the model is mainly used for evaluation of design rather than operational optimisation studies. OTTER contains models for most commonly encountered processes and less conventional processes may require development of a suitable mathematical model (Butt and Head, 2002). OTTER is a well-developed model for design purposes in particular, but has a closed structure. It is difficult to develop process models in this environment and knowledge exchange is hampered. Metrex is being developed mainly for particle removal, but has as an advantage that it is written in an accessible language and exchange and development is easy. With TAPWAT stochastic and simple process modelling can be performed for pathogenic micro-organism removal and disinfection by-product formation. The model is not intensively tested and still in a development phase. It is not used outside RIVM.

Also several isolated modelling efforts are made to optimise operation of drinking water treatment processes. The models are mostly data-driven and concentrate on the floc formation process (Wistrom and Farrel, 1998; Zang and Stanley, 1999; Baxter, 1999; Baxter et al., 2001; Baxter et al., 2002; Yu et al., 2000). The drawback of data-driven models, however, is that the application cannot be generalised. It is problematic to predict outside the calibration/validation range, let alone to use the developed models for evaluation of new designs. In addition, it is difficult to incorporate existing knowledge into the data-driven models or to extract information from these models.

In order to be able to use models for improving the operation of drinking water treatment processes and to cope with the drawbacks of the existing models, the Stimela environment, with phenomenological, dynamic models describing the process based on partial differential equations (see chapter 2), is being developed. In summary Stimela aims to address the requirements of different target groups. A summary is given in table 3.2.

Table 3.2 Summary of modelling requirements for different uses

	Operation	Research	Design	Education/training
Flexible programming		x		
Process interactions	x			
Visualisation	x	x	x	x
Calibration	x	x	x	x
Analysis	x		x	x
Control	x			
Demonstration				x

Stimela incorporates typical Dutch developments in the platform, such as GAC filtration in combination with ozonation, biological nitrification and softening by pellet reactors. The knowledge of drinking water treatment in the Netherlands is gradually added to the software and with Internet application it is made accessible.

3.5.2 Description of Stimela

Stimela is an environment where different drinking water treatment processes can dynamically be modelled. The Stimela models are developed in Matlab/Simulink™. Partial differential equations (see chapter 2) are numerically integrated with the consequence that variations in time and space can be followed. The models of individual processes are situated in a model library and can be connected to each other, forming a complete treatment train (see figure 3.3). In this way, the effect of operational changes in preceding treatment processes can be evaluated. Because Matlab/Simulink™ is used, the models are easily accessible, the structure is open and flexible and all routines, toolboxes and visualisation techniques of Matlab/Simulink™ can be used (Helm and Rietveld, 2002).

A Stimela model consists of an input block, one or more process blocks, control blocks and graphical output blocks. By opening the input block, values for the raw water quality and the flow can be inserted. These can be constant values, but also a file can be uploaded in which the changes of the raw water quality parameters in time are given. The connecting line between blocks transfers the values of the water quality parameters at every time step. By opening the process block, design, and calibration parameters can be inserted. The design parameters determine the process physically and are not changed in time. Calibration parameters are determined by the prevailing circumstances and must be obtained by additional experiments. Calibration is executed with obtained measurement data of a pilot or full-scale plant. Calibration parameters can be floc density, filtration coefficient, Freundlich-constants, gas transfer coefficient, etc.

In addition to the input block, the process block can also be fed by a control block. The control block gives values for the manipulated parameters to the process block. These values can change in time depending on the (required) control action.

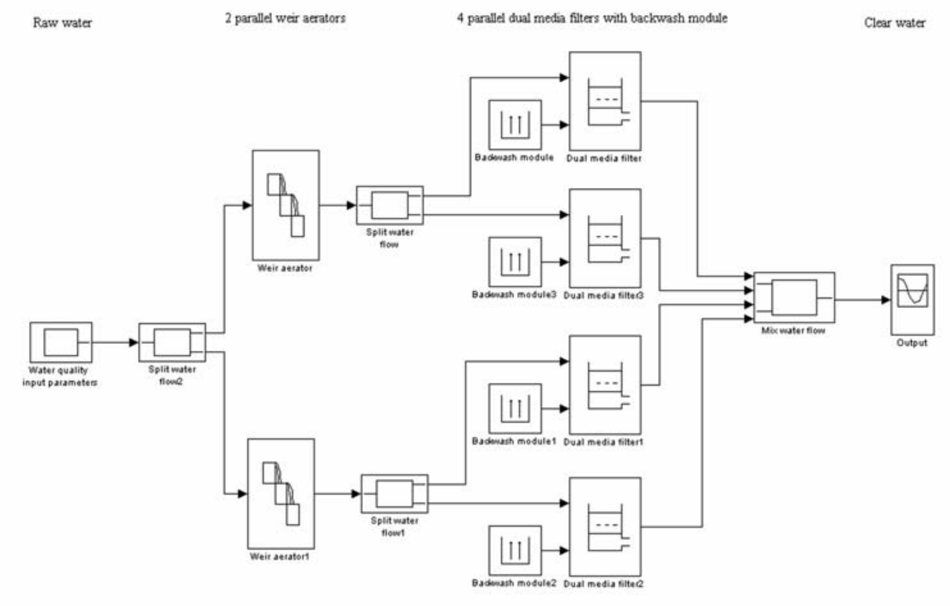


Figure 3.3 Example of a treatment train in Stimela environment

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

3.5.3 Numerical integration, schematising the reactor

In order to be able to solve the partial differential equations numerically with Matlab/Simulink™, they must be transferred to a set of ordinary differential equations (ODE's). This is done by discretising the reactor to space, using unit elements (see figure 3.4).

An advection-dispersion flow in a tank behaves as if the tank were compartmentalised. When the advection term is described by means of Taylor expansion (Peyret and Taylor, 1983):

$$\frac{dc_1}{dx} = \frac{c_1 - c_0}{\Delta x} + \frac{\Delta x}{2}\frac{d^2 c}{dx^2} + ...$$

A plug flow can be described as follows:

$$\frac{\partial c_1}{dt} = -u\frac{\partial c_1}{dx} = -u(\frac{c_1 - c_0}{\Delta x} + \frac{\Delta x}{2}\frac{\partial^2 c_1}{\partial x^2})$$

The last term is the discretisation error, also called numerical dispersion. Comparing the equation with the equation for advection and dispersion and when $u\Delta x/2 = D_x$, numerical dispersion is equal to physical dispersion and can thus be used to describe real flow conditions. The equation for transport is thus written as a tank-in-series model, considering the unit element as a continuous stirred tank reactor (CSTR). The more unit elements the better a plug flow is approached.

The basic discrete equations of a treatment process, neglecting degradation in the water phase and transport and degradation in the solid or gas phase, are then given in the following ordinary differential equations (ODEs) (based on Euler):

$$\frac{dc_1}{dt} = -u\frac{c_1 - c_0}{\Delta x} - k_2(c_{e1} - c_1)$$

$$\frac{dc_{g,s1}}{dt} = -u\frac{c_1 - c_0}{\Delta x}$$

Where:

Δx	height of unit element (m)
c_0	influent concentration (g/m^3)
c_1	effluent concentration (g/m^3)
c_e	equilibrium concentration (g/m^3)
u	(superficial) flow velocity through reactor (m/s)
k_2	transfer rate (s^{-1})

For a combination of three unit elements in series the system of ODEs becomes:

$$\begin{pmatrix} \dfrac{dc_1}{dt} \\ \dfrac{dc_2}{dt} \\ \dfrac{dc_3}{dt} \end{pmatrix} = \frac{u}{\Delta x} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix} - k_2 . \begin{pmatrix} c_{e1} - c_1 \\ c_{e2} - c_2 \\ c_{e3} - c_3 \end{pmatrix}$$

$$\begin{pmatrix} \dfrac{dc_{g,s_1}}{dt} \\ \dfrac{dc_{g,s_2}}{dt} \\ \dfrac{dc_{g,s_3}}{dt} \end{pmatrix} = \frac{u}{\Delta x} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

Matlab/Simulink™ provides a number of solvers for the simulation of such equations. Because of the diversity of dynamic system behaviour, some solvers may be more efficient than others at solving particular problems. One can choose between variable-step and fixed-step solvers. The ODE solver functions implement numerical integration methods for solving initial value problems for ODEs. Beginning at the initial time with initial conditions, they step through the time interval, computing a solution at each time step. If the solution for a time step satisfies the solver's error tolerance criteria, it is a successful step. Otherwise, it is a failed attempt and the solver shrinks the step size and tries again (The Mathworks, 1999).

3.5.4 Set-up of the Stimela model

The model of a process in Stimela consists basically of 6 files (DHV, 1999). In the initialisation file, the number of input parameters, output parameters and ODEs are defined. In addition, the water quality parameters that are of interest in the process are given. In the parameter file the process parameters that are given in the process block are processed. The system file (s-function) is the heart of the model. In this file the ODEs are given in matrix notation. In addition, the output parameters are defined. The graphical output file gives the possibility for visualisation of the output from the numerical integration. The remaining two files determine the graphical interface for insertion of process parameters.

3.5.5 Example of modelling rapid sand filtration

To illustrate the set-up and the use of Stimela, an example of modelling of rapid filtration is given. The main purpose of rapid filtration is the removal of suspended solids. The suspended solids accumulate in the filter until the maximum head loss is reached and the filter must be backwashed.

The following parameters have to be inserted:

- Water parameters: flow, suspended solids concentration, temperature
- Design parameters: surface area, bed height, grain size, porosity, supernatant water height
- Calibration parameters: clean bed filtration coefficient, floc density, maximum pore filling

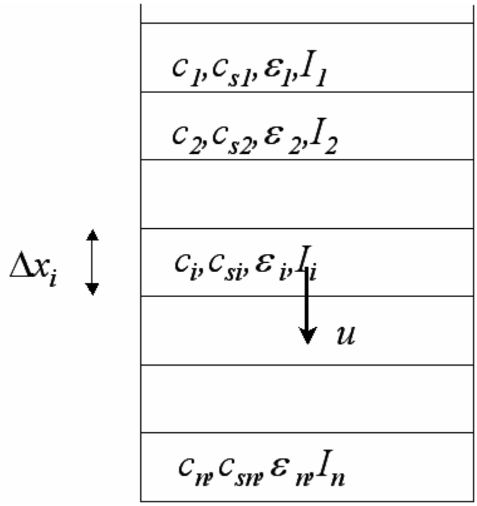


Figure 3.4 Schematic representation of filter bed

In this example the mathematical description of the process is based on Maroudas' equation for filtration and Carman Kozeny's equation for head loss calculation in de filter bed. The filter bed is subdivided into *n* unit elements (see figure 3.4) and per unit element *i* per time step the different parameters are calculated.

The suspended solids concentration in the i^{th} unit element is the inflow for the subsequent element $i+1$. The suspended solids concentration of the n^{th} element is the concentration leaving the filter bed and can be compared with measured effluent concentrations.
The head loss over a unit element is the head loss gradient (I_i) times the height of the element (Δx).
The sum of the head losses of the unit elements is the total head loss over the filter bed. With the values for head loss, a Lindquist diagram can be drawn, representing the head loss build up over the filter bed in time (see figure 3.5).

The discrete equations for unit element *i* is presented by:

$$\frac{dc_i}{dt} = -\frac{u}{\varepsilon_i}\frac{c_i - c_{i-1}}{\Delta x} - k_{2i}c_i(1 - \frac{c_{si}}{\rho_d \varepsilon_0 \zeta})$$

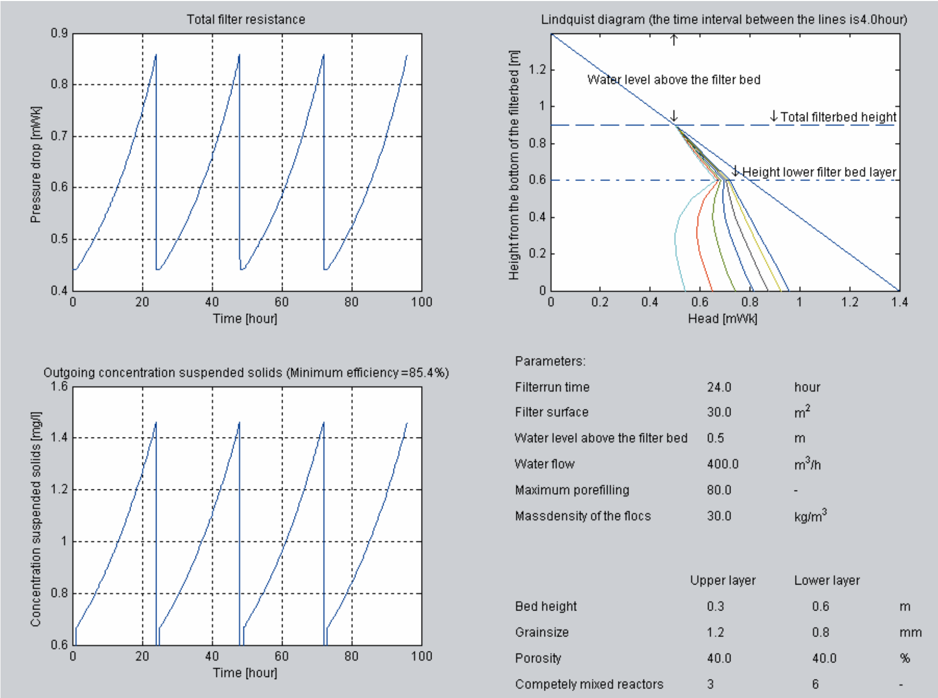
$$\frac{dc_{si}}{dt} = -u\frac{c_i - c_{i-1}}{\Delta x}$$

$$I_i = I_0(\frac{\varepsilon_0}{\varepsilon_0 - \frac{c_{si}}{\rho_d}})^2$$

$$I_0 = 180\frac{\nu}{g}\frac{(1-\varepsilon_0)^2}{\varepsilon_0{}^3}\frac{v}{d_0{}^2}$$

Where

ζ	maximum pore filling (-)
c_i	suspended solids concentration (g/m^3)
c_{si}	concentration of accumulated solids in filter (g/m^3)
ε_i	porosity (-)
I_i	head loss gradient over unit element (-)
k_{2i}	transfer coefficient (s^{-1})



Parameters:

Filterrun time	24.0	hour
Filter surface	30.0	m^2
Water level above the filter bed	0.5	m
Water flow	400.0	m^3/h
Maximum porefilling	80.0	-
Massdensity of the flocs	30.0	kg/m^3

	Upper layer	Lower layer	
Bed height	0.3	0.6	m
Grainsize	1.2	0.8	mm
Porosity	40.0	40.0	%
Competely mixed reactors	3	6	-

Figure 3.5 Graphical output of simulation of (dual media) filtration

3.6 Internet application of Stimela

For the use of models to evaluate the data from drinking water treatment plants (and pilot plants) a website is being developed where Stimela models can be approached and communication about the results can occur (www.stimela.com).
The website consists of a home page where the following items are presented:

- Introduction to Stimela website and user management system
- Explanation and visualisation of drinking water treatment processes
- Design exercise for education and explanation of use of models
- Communication platform for exchange with other users and model developers
- Gateway to Stimela simulations

Introduction. In the introduction the Stimela site is further explained. In addition, user management is performed and registration occurs. Users will not be asked for payment, but for the communication it is of importance that the users are serious and recognisable.

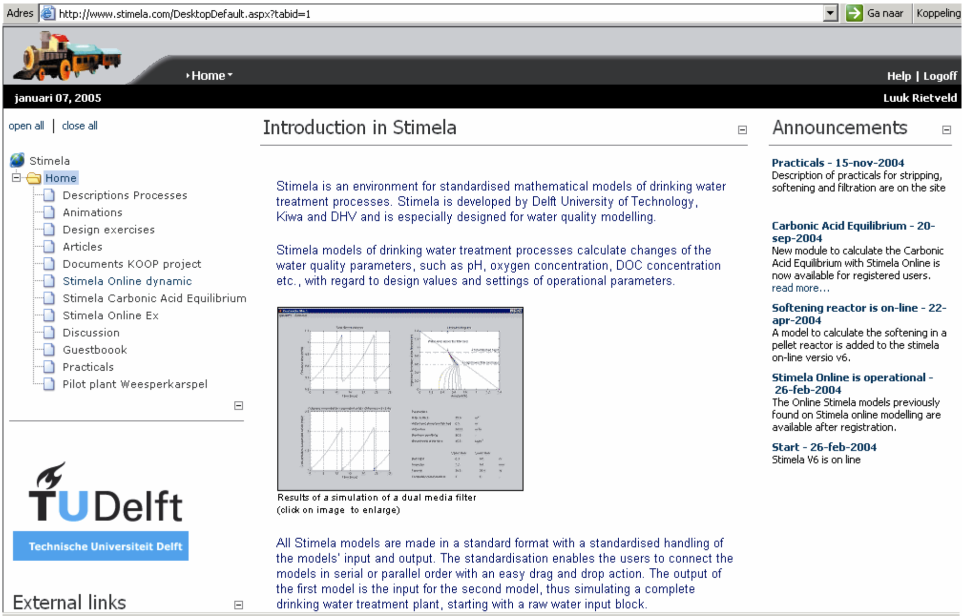
Treatment processes. For education and training the treatment processes are described. The descriptions are based on the lecture notes used for educational purposes at Delft University of Technology.

Design exercise. To illustrate the design procedure, a design exercise is included that is used by final year students in sanitary engineering at Delft University of Technology. They are asked to design an additional process in an existing plant to improve water quality. Therefore, they generate alternatives, study the treatment, process, main water flow and hydraulic line schemes and come up with a solution. To calculate the dimensions of the new process they need computer models. With the models they can also evaluate the flexibility of the process with respect to operational changes. On the website several of these exercises are shown and the use of models is explained. The design exercise can also function as a tutorial for other users.

Communication. The main purpose of the website is to communicate about drinking water treatment modelling. Therefore, the results of calculations will be represented in a report. Depending on the user the reports are either open for other users or the information will remain protected. The more reports will be generated, the more exchange of information and knowledge between users will occur. In the communication section it is also possible to ask support from other users or from the model developers.

Stimela simulations. From the home page the Stimela simulation site can be approached. Here individual processes can be modelled. Standard raw water data can be used or specific raw water quality data can be imported. The process parameters are subdivided into design, calibration and control parameters. After specifying the design characteristics of the process, the plant can be simulated for different set-points of the control parameters. The results are given in a graphical output and are compared to drinking water quality guidelines. After finishing the calculations, a report is generated that is sent to the communication section.

In figure 3.6 and 3.7 examples are given of how the models can be approached.



Introduction in Stimela

Stimela is an environment for standardised mathematical models of drinking water treatment processes. Stimela is developed by Delft University of Technology, Kiwa and DHV and is especially designed for water quality modelling.

Stimela models of drinking water treatment processes calculate changes of the water quality parameters, such as pH, oxygen concentration, DOC concentration etc., with regard to design values and settings of operational parameters.

Results of a simulation of a dual media filter
(click on image to enlarge)

All Stimela models are made in a standard format with a standardised handling of the models' input and output. The standardisation enables the users to connect the models in serial or parallel order with an easy drag and drop action. The output of the first model is the input for the second model, thus simulating a complete drinking water treatment plant, starting with a raw water input block.

Announcements

Practicals - 15-nov-2004
Description of practicals for stripping, softening and filtration are on the site

Carbonic Acid Equilibrium - 20-sep-2004
New module to calculate the Carbonic Acid Equilibrium with Stimela Online is now available for registered users.
read more...

Softening reactor is on-line - 22-apr-2004
A model to calculate the softening in a pellet reactor is added to the stimela on-line versio v6.

Stimela Online is operational - 26-feb-2004
The Online Stimela models previously found on Stimela online modelling are available after registration.

Start - 26-feb-2004
Stimela V6 is on line

Figure 3.6 Introduction page of website www.stimela.com

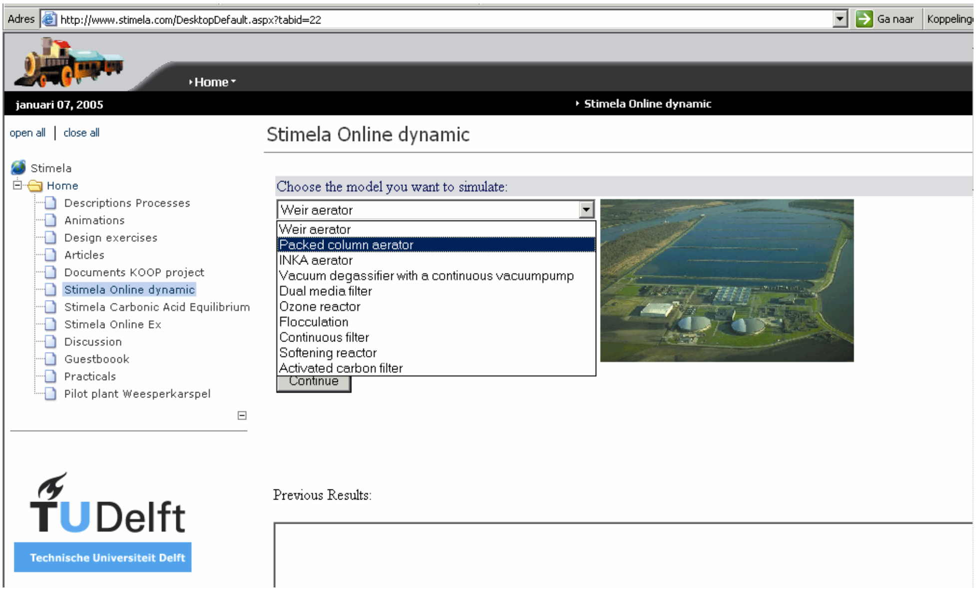


Figure 3.7 Modelling page on web site www.stimela.com

3.7 Modelling approach

Experiments in pilot plants at drinking water treatment plants are generally executed to prove the robustness of the process and the fact that product water quality meets the guidelines under all circumstances. In addition, full-scale plants are monitored for checking the drinking water quality and the performance of individual processes. Sometimes, incidental laboratory tests are executed for fundamental research. To come to improvement of operation of drinking water treatment processes, maximal use of obtained information should be made and therefore, the data should be integrated and evaluated by models.

In turn the calibration and validation of models asks for specific information from the laboratory and pilot and full-scale installations. Models, thus, can give input to the testing and monitoring programmes (experiment design), resulting in more efficient testing with increased knowledge about the process.

When modelling is used for improvement of operation, experiments for calibration and validation should be executed in a structured way.

First of all literature should be studied to identify possible benefits for operational improvements of the process, to define the partial differential equations that describe the process and to make a first estimate of the calibration parameters. With the model, existing data (from pilot and full-scale plants) are evaluated and parameter identification is started-up. Normally, this will result in a set-up of a testing programme for additional experiments.Using the model for evaluating the testing programme, it can be made efficient, without superfluous measurements.

When the model is calibrated and validated, simulation of the actual operation of the system can be performed. By repeating this process for the various alternative operational scenarios of the system, and by comparing their performance, most promising scenarios can be identified. The experiments are then done on the model rather than on the real system itself only because the latter would be too inconvenient, expensive, and time-consuming (Hillier and Lierbermann, 1995). The best alternative is implemented for operation of the treatment process. During application of the model, data are continuously collected and used for on-line parameter identification, improving the quality of the model and its field for application.

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4 DETERMINATION OF CT-VALUE OF OZONE BUBBLE COLUMNS

4.1 Introduction

In drinking water treatment ozonation is one of the main barriers for pathogenic micro-organisms. Ozone is normally dosed in bubble columns and, afterwards, the water flows through contact chambers where the reactions can take place. During ozonation, the CT-value is a leading parameter to determine the decimal elimination capacity (DEC). The CT-value is normally determined for the contact chambers and the effect of the bubble column, where the ozone is added, is neglected. Therefore, the disinfection capacity of the ozone installation is underestimated and/or overdosing of ozone occurs.

Figure 4.1 Ozone generator at Amsterdam Water Supply

To determine a CT-value for the total installation that can be translated to a realistic disinfection capacity, the ozone profile in the bubble column should also be determined. This can be achieved by modelling the ozone concentration, supported by incidental sampling programmes.

In this chapter a model for the determination of the ozone concentration in a bubble column is presented and calibrated. The model is based on a phenomenological description of the processes inside the reactor. The processes are advection and dispersion of the water flowing through the bubble column, ozone mass transfer from the gas phase to the water, slow decay of ozone and competitive reactivity of constituents in water with dissolved ozone (rapid decay of ozone) (Zhou et al., 1994, El-Din and Smith, 2001). The kinetic reaction of ozone follows a complex mechanism, the consumption of ozone by water depends on the water quality parameters such as temperature, pH, alkalinity, organic matter (Roustan et al.,1996).

Most of the processes are fairly well documented in literature, except for the rapid decay of ozone in natural water. Therefore, in this chapter special attention is paid to this element.

In the pilot plant Weesperkarspel of Amsterdam Water Supply, separate tests are carried out for the determination the slow decay of ozone. The rapid decay is determined from the calibration of the model to sampling data of a co-current and counter current flow reactor.

4.2 Modelling of ozone in water and gas

4.2.1 Transport of ozone through a reactor in water

In case of stationary water and gas flows in an ozone aerator, where dispersion is neglected and decay only occurs in the water, the overall equations for transport in the water and the gas phase (see chapter 2)

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_g) = 0$$

$$\frac{\partial c_g}{\partial t} - D_{x,g} \frac{\partial^2 c_g}{\partial x^2} + u_g \frac{\partial c_g}{\partial x} + f_{1,g}(c_g) + f_{2,g}(c, c_g) = 0$$

are reduced to:

$$u \frac{dc_{O3}}{dx} + f_1(c_{O3}) + f_2(c_{O3}, c_{g,O3}) = 0$$

$$u_g \frac{dc_{g,O3}}{dx} + f_{2,g}(c_{O3}, c_{g,O3}) = 0$$

The mass balance (not taking decay into account) between the water and gas phase can be written as:

$$\alpha\, Q_g \frac{dc_{g,O3}}{dx} = -Q \frac{dc_{O3}}{dx} \Rightarrow \frac{dc_{g,O3}}{dx} = -\frac{1}{\alpha} \frac{Q}{Q_g} \frac{dc_{O3}}{dx} = -\frac{1}{\alpha} \frac{1}{RQ} \frac{dc_{O3}}{dx}$$

The pressure factor (α) is introduced, because the ozone concentration in the gas phase is expressed in g/Nm^3. Bubble columns are high (about 4 m) and the pressure at the bottom of the column is significantly higher than atmospheric. Therefore, the gas concentration c_g must be multiplied by the correction factor α.

The change in gas concentration in the gas phase will result in an opposite change in gas concentration in the water. Inserting this relation into the equation for gas transport in the water and the gas phase, the relation between the transfer rates from the water and from the gas phase is found:

$$\left.\begin{aligned} u\frac{dc_{O3}}{dx} &= -f_2(c_{O3},c_{g,O3}) \\ u_g\frac{dc_{g,O3}}{dx} &= f_{2,g,s}(c_{O3},c_{g,O3}) \end{aligned}\right\} \Rightarrow f_{2,g}(c_{O3},c_{g,O3}) = -u_g\frac{1}{RQ}\frac{\partial c_{O3}}{\partial x} = \frac{u_g}{u}\frac{1}{\alpha}\frac{1}{RQ}f_2(c_{O3},c_{g,O3})$$

Where

RQ	gas to water flow ratio (Q_g/Q) (Nm^3/m^3)
Q, Q_g	water flow (m^3/s) and gas flow (Nm^3/s) respectively
u, u_g	water velocity (m/s) and gas velocity (Nm/s) respectively
c_{O3}, $c_{g,O3}$	ozone concentration in water(g/m^3) and gas (g/Nm^3) respectively
D_x, $D_{g,x}$	dispersion coefficient in water and gas respectively (m^2/s)
α	pressure and temperature correction factor $\alpha=(P_g/P_0)(T_0/T_g)$
P_0 P_g	standard and actual pressure (Pa) respectively
T_0 T_g	standard and actual temperature (K) respectively.

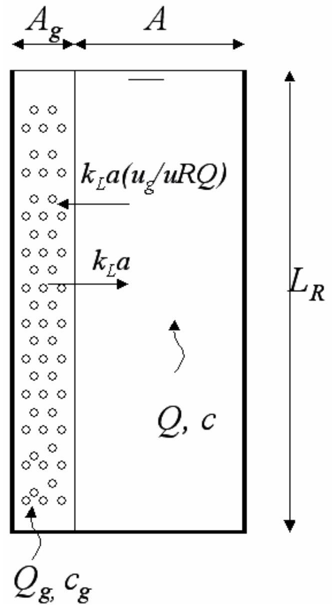

Figure 4.2 Impression of ozone bubble column

The gas velocity u_g is dependent on the direction of the flows. With co-current flow $u_g = u_b+u$ (Wallis, 1969).

It is now necessary to find a relation for the decay (f_1) and transfer components (f_2) of the equations.

4.2.2 Transfer of ozone from gas phase to water

If water is exposed to a gas mixture containing ozone a continuous exchange of ozone molecules takes place from the water into the gas phase and vice versa. As soon as the equilibrium concentration in the water is reached both mass transfers will be of equal magnitude such that no overall change of the ozone concentrations in water and gas phase occurs. The saturation concentration increases with increasing ozone concentration in the gas phase. The relation between the saturation concentration and gas concentration in the gas phase is linear (Mueller et al., 2002):

$$c_{e,O3} = \alpha\, K_D c_{g,O3}$$

Where

$c_{e,O3,}$	equilibrium concentration of ozone in water (g/m^3)
$c_{g,O3}$	concentration of ozone in gas phase (g/Nm^3)
K_D	distribution coefficient (-)

The mass transport in the water phase is defined by Fick's law, assuming that the water concentration in the bulk water is uniform and the concentration gradient only occurs in a laminar water film near to the interface, the equation can be written as (James, 1993):

$$\frac{dc_{O3}}{dt} = D_{O3}\frac{A_I}{V}\frac{(c_{e,O3} - c_{)3})}{d_L} = k_L a(c_{e,O3} - c_{O3})$$

where

A_I	interfacial area (m^2)
V	volume of water (m^3)
D_{O3}	diffusion coefficient of ozone (m^2/s)
k_L	transfer coefficient (m/s)
a	specific surface area (1/m)
d_L	thickness of water film (m)

In a bubble column, the specific surface area of the bubbles can be calculated as follows:

$$\left.\begin{aligned} & A_{Ib} = V_b \frac{6}{d_b} \\ & a = \frac{A_{Ib}}{V} \\ & \frac{V_g}{V} = \frac{Q_g / u_g}{Q_w / u} = RQ \frac{u}{u_g} \Rightarrow V_g = RQ \frac{u}{u_g} V \end{aligned}\right\} a = \frac{RQ \frac{u}{u_g} V \frac{6}{d_b}}{V} = RQ \frac{u}{u_g} \frac{6}{d_b} = h \frac{6}{d_b}$$

Where

A_{Ib} total surface area of bubbles in the reactor (m^2)

V_g total bubble volume in reactor (m^3)

d_b bubble diameter (m)

h gas hold-up (-).

For the k_L -value different expressions are elaborated. The best-known expression is given by Hughmark (1967).

$$k_L = \frac{D_{O3}}{d_b} \left(2 + 0.061 \left[\left(\frac{u_b d}{\nu} \right)^{0.48} \left(\frac{\nu}{D_{O3}} \right)^{0.34} \left(\frac{d_b g^{0.33}}{D_{O3}^{0.66}} \right)^{0.072} \right]^{1.61} \right) \quad \text{for single gas bubbles}$$

$$k_L = \frac{D_{O3}}{d_b} \left(2 + 0.0187 \left[\left(\frac{u_b d}{\nu} \right)^{0.48} \left(\frac{\nu}{D_{O3}} \right)^{0.34} \left(\frac{d_b g^{0.33}}{D_{O3}^{0.66}} \right)^{0.072} \right]^{1.61} \right) \quad \text{for swarms of gas bubbles}$$

Where

ν kinematic viscosity (m^2/s)

The bubble diameter is dependent on the type of diffusers. Roustan et al. (1996) used a photographic technique to measure the bubble size distribution and gas hold-up in a pilot bubble ozone column. The authors found that in the dispersed bubble regime, the bubble size distribution varied from 1.75 to 5.25 mm. Langlais et al. (1991) suggested that ozonation systems should be designed to generate the gas bubbles with a mean diameter around 1 to 3 mm. These diameters are also observed in the study of Zhou and Smith (2000) using a particle dynamics analyser. The bubble sizes will not be constant over the height of the reactor. Due to coalescence and break-up the bubble size distribution will change (Shimizu et. al, 2000). In addition, the volume of the bubbles will increase as the pressure on the bubbles drops (on the top of the column), while due to gas transfer from the bubbles the size will decrease.

The rising velocity of a bubble (u_b) in stagnant water is dependent on the radius of the bubble (Wallis, 1969). For (small) bubbles the following relation can be applied:

$$u_b = 0.0135\left(\frac{20000\sigma}{\rho_w d_b}\right)^{0.5}$$

Where

σ surface tension (N/m)

ρ_w water density (kg/m^3)

4.2.3 Decay of ozone

The decay of ozone in water has been investigated by several researchers. According to Park et al. (2001), ozone, added to natural water, is consumed in two steps: the rapid ozone consumption step and the rather slow decay step. The amount of ozone consumed during the first stage can be represented by the parameter ID (Instantaneous ozone Demand) that corresponds to the difference between the administered ozone and the amount of ozone measured after a few seconds. The slower decay is kinetically first order and affected by pH, ultraviolet light, ozone concentration and the concentration of radical scavengers (Langlais, 1991). One of the causes of ID is Natural Organic Matter (NOM). The instantaneous ozone demand can also be explained by the enhancement of the mass transfer from gas phase into water phase due to rapid chemical reactions (Danckwerts, 1970). To quantify this enhancement, an enhancement factor k_E was defined as the actual rate of mass transfer with the occurrence of chemical reactions divided by the maximum rate of physical absorption without any chemical reaction. The enhancement factor is in between 2 and 8, depending on the water quality. Taking the considerations stated above into account, the differential equation for ozone transfer and decay in water can be written as follows:

$$\frac{dc_{O3}}{dt} = \frac{k_L}{k_E} RQ \frac{u}{u_g} \frac{6}{d_b} (\alpha K_D c_{g,O3} - c_{O3}) - k_{O3} c_{O3}$$

or

$$\frac{dc_{O3}}{dt} = (1 - k_{ID}) k_L RQ \frac{u}{u_g} \frac{6}{d_b} (\alpha K_D c_{g,O3} - c_{O3}) - k_{O3} c_{O3}$$

Where

k_{O3} slow ozone decay rate (s^{-1})

k_{ID} instantaneous ozone demand factor (-)

The first term on the right represents the transfer of ozone to water influenced by instantaneous ozone demand, while the second term represents the slow decay of ozone in water.

According to Yurteri and Gurol (1998), the decay can be expressed as:

$$k_{O3}c = \sum_i k_i c_i$$
$$k_i = (k_{d_i} + k_{r_i}\psi_i)$$

where c_i is the concentration of substrate i in water and k_i is the apparent reaction rate constant for c_i. The apparent reaction rate constant consists of two terms, which reflect direct (k_{di}) and radical (k_{ri}) reactions of ozone with organic matter. The factor ψ_i accounts for initiation and scavenging of radical reactions. Yavich and Masten (2001) stated that NOM is a complex matrix of organic materials and a simpler approach to describing the reaction of ozone with NOM must be identified. Suggested was to use two surrogate parameters for organic matter, humic and nonhumic fraction of NOM.

From practice it is known that direct consumption of ozone is greater when the UV absorbance of humic substances is higher and that during the ozonation process a strong degradation of UV absorbance occurs (Langlais, 1991). Therefore, in this chapter the instantaneous ozone demand is described as function of the degradation of UV absorbance, resulting into the following equation:

$$\frac{dc_{O3}}{dt} = -\frac{k_{UV}}{Y}(UV - UV_0)c_{O3} - k_{O3}c_{O3}$$
$$\frac{d(UV)}{dt} = -k_{UV}(UV - UV_0)c_{O3}$$

Where

UV	UV absorbance (254 nm) in water (m^{-1})
UV_0	stable UV absorbance (254 nm) after completion of the ozonation process (m^{-1})
Y	yield factor (m^4/g)
k_{UV}	decay coefficient of UV absorbance ($m^3/g.s$)

The first term of the first equation indicates the rapid decay of ozone in water. It is assumed that not all UV absorbance is degraded, but, after ozonation, a stable UV absorbance exists. This stable UV absorbance (UV_0) is incorporated in the equation. As the ozonation progresses, the rate of ozone decay is shifted to the slow kinetic regime (Zhou and Smith, 2000). The second term of the first equation indicates the slow decay of ozone in water. Slow decay can be determined by taking a water sample from a bubble column and analysing the ozone concentration at regular intervals. Rapid decay or instantaneous ozone demand is determined by calibration of the model on pilot plant data of ozone concentration over the height of the bubble column.

4.2.4 General equation for transport, transfer and decay of ozone

Assuming a water and gas transport without dispersion, neglecting decay of ozone in the gas phase and filling in the relations of equilibrium, transfer and decay, the equations for ozonation in a bubble column are given by:

$$\frac{\partial c_{O3}}{\partial t} = -\frac{Q}{A}\frac{\partial c_{O3}}{\partial x} + k_L RQ \frac{u}{u_g}\frac{6}{d_b}(\alpha K_D c_g - c_{O3}) - k_{O3}c_{O3} - \frac{k_{UV}}{Y}(UV - UV_0)c_{O3}$$

$$\frac{\partial c_{g,O3}}{\partial t} = -\frac{Q_g}{hA}\frac{\partial c_{g,O3}}{\partial x} + \frac{k_L}{\alpha}\frac{6}{d_b}(\alpha K_D c_{g,O3} - c_{O3})$$

$$\frac{\partial (UV)}{\partial t} = -\frac{Q}{A}\frac{\partial (UV)}{\partial x} - k_{UV}(UV - UV_0)c_{O3}$$

4.3 Materials and methods

4.3.1 Modelling approach

The model is developed within the Stimela environment (see chapter 3).

The model consists of:

- Input disturbance variables:
    - water flow Q (m^3/s)
    - water temperature T (K)
    - ozone concentration c_{O3} (g/m^3)
    - UV absorbance (m^{-1})
- Input manipulated variables:
    - concentration of ozone in gas $c_{g,O3}$ (g/Nm^3)
    - gas flow Q_g (Nm^3/s)
- State variables:
    - ozone concentration c_{O3} (g/m^3)
    - concentration of ozone in gas $c_{g,O3}$ (g/Nm^3)
    - UV absorbance (m^{-1})
- Output water quality variables:
    - water flow Q (m^3/s)
    - water temperature T (K)
    - ozone concentration c_{O3} (g/m^3)
    - UV absorbance (m^{-1})
- Extra output variables:
    - ozone concentration over the height of the reactor

    - concentration of ozone in gas over the height of the reactor
- Physical parameters:
    - surface area of reactor A_T (m^2)
    - column height L_R (m)
    - distribution coefficient K_D
    - direction of water flow
    - bubble diameter d_b (m)
    - transfer coefficient k_L (m/s)
    - gas hold-up h (-)
- Calibration parameters
    - decay coefficients k_{O3} (s^{-1}) and k_{UV} (m^3/g.s)
    - Yield factor (m^4/g)
    - number of unit elements (-)

At start-up of the reactor (initial condition) the ozone concentration, the concentration of ozone in gas and the UV absorbance is equal to the input concentration.

4.3.2 Description of pilot plant Weesperkarspel of Amsterdam Water Supply

The model for simulating the ozone bubble column was tested on data from bubble columns of the pilot plant Weesperkarspel of Amsterdam Water Supply (see figure 4.3). The columns of the pilot plant have a diameter of 0.1 m and a height of 6 m and are made of perspex. The water for the pilot installation is taken from the main water stream of the drinking water treatment plant and is stored in a 10 m^3 tank. In case of a co-current flow the effluent water is collected at a height of 4.95 m from the gas injection point in the tank. In case of a counter current the effective height of the column is 4.4 m. The water flow in the bubble columns can be varied between 0 and 1.5 m^3/h and the gas flow between 0 and 0.1 Nm^3/h.

From the pilot plant the slow decay rate of ozone was measured separately. The calibration of the decay coefficient of ozone is determined by taking samples from the bottom of a counter current flow column. Different ozone doses were applied (1.86, 2,46 and 3.25 g/m^3) to determine the decay coefficient under different initial concentrations. The samples are stored and the ozone concentration in water is measured after different residence times (0, 30, 60, 90, 120, 150, 180, 210 and 240 s).

Figure 4.3 Pilot plant with ozone bubble columns

The model for simulating the ozone bubble column was developed within the Stimela environment (see chapter 3). The calibration of the model was executed and the influence of instantaneous ozone demand (rapid decay) on the ozone concentration in water was determined by using a bubble column in co-current and counter current flow. Under an ozone dose of 3.5 g/m^3, where the water flow is Q_w=0.65 m^3/h (82.8 m/h) and the gas flow Q_g=0.1 Nm^3/h (12.7 Nm/h), the ozone concentration was measured over the height of the column. The temperature of the water was 20 ^{o}C and the Dissolved Organic Carbon concentration (DOC) was about 6 mg C/l. The influent UV absorbance was about 14/m and the effuent about 7/m. It is assumed that bubble size is constant (d_b=3 10^{-3} m), ideal plug flow occurs and k_L-value is 3 10^{-4} m/s. It is further assumed that the calibration parameters for rapid decay k_{UV} and Y must be the same for both bubble column configurations.

Ozone in water is measured using DPD-sulphate in the presence of Potassium Iodide. The extinction of colour is determined with an UV/VIS-spectro-photometer at 550 nm.

4.4 Determination of calibration parameters

4.4.1 Slow decay of ozone in water

The results of the determination of the slow decay rate of ozone k_{O3} are presented in figure 4.4. During the tests a stable concentration of ozone was measured at the end of the experiment. Therefore all data were corrected with 0.028 g/m^3. From the graphs it can be concluded that the decay coefficient is dependent on the initial ozone dose. The highest ozone dose (3.25 g/m^3) gives the lowest coefficient for slow decay. This is conform the observations of Park et al. (2001). The lower ozone doses (2.46 and 1.86 g/m^3) give similar decay coefficients. In the calculations, the slow decay rate k_{O3} is taken as 0.014/s, assuming that with the high ozone dose no interference with rapid decay exists.

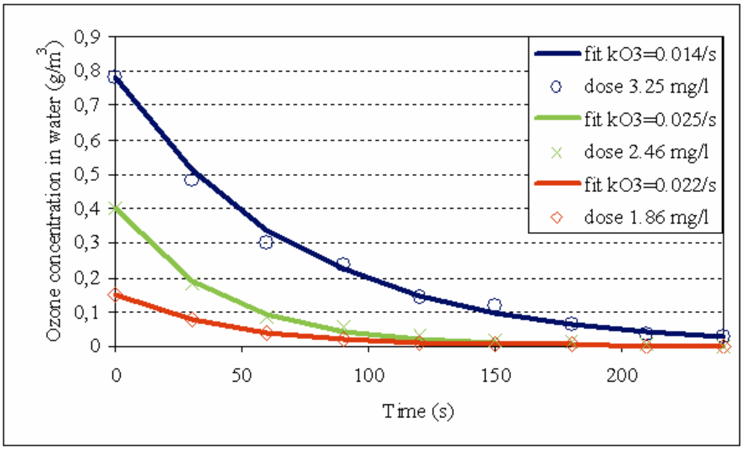

Figure 4.4 Slow decay of ozone at different ozone doses

4.4.2 Rapid decay of ozone in water

In figure 4.5 and 4.6 the ozone concentration in water is given for the co-current and counter current flow column respectively. The water flow in figure 4.5 is represented from left to right and in figure 4.6 from right to left. If the instantaneous ozone demand is neglected, the ozone concentration in the water is overestimated (red line). Introducing the additional term that accounts for the instantaneous ozone demand following the concept of Park et al. (2001), the ozone concentration in water is now underestimated at upstream parts of the bubble column (green line). Better results are obtained with the calibration of the model that incorporates the degradation of UV absorbance. During the process in the bubble column UV absorbance is degraded and the ozone concentration in the upstream parts of the reactor are better predicted (blue line). The relative UV absorbance is represented by a dotted line and decreases in the direction of the flow from 1 to (almost) 0.

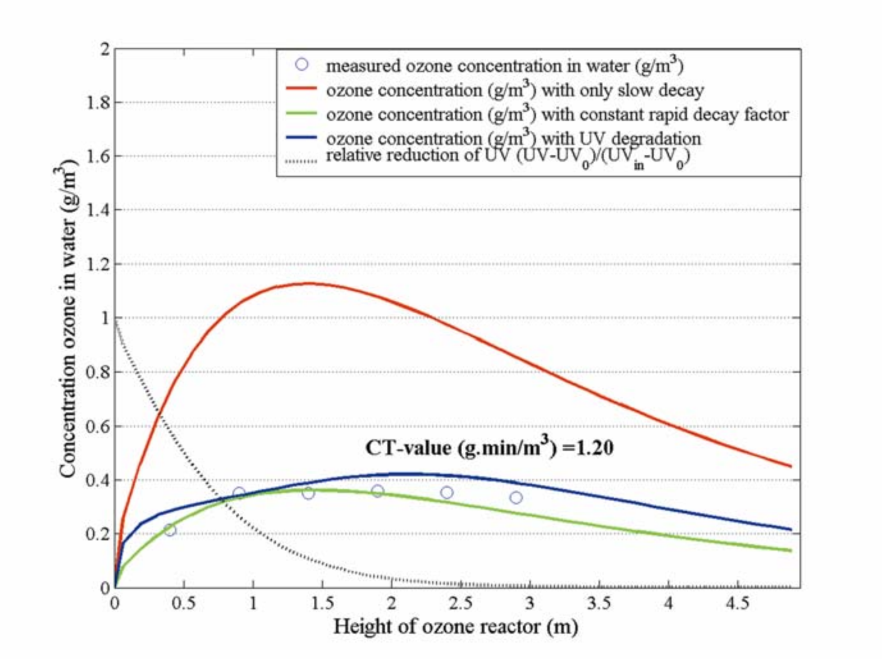

Figure 4.5 Model calibration of co-current flow ozone and ozone dose of 3.5 g/m^3

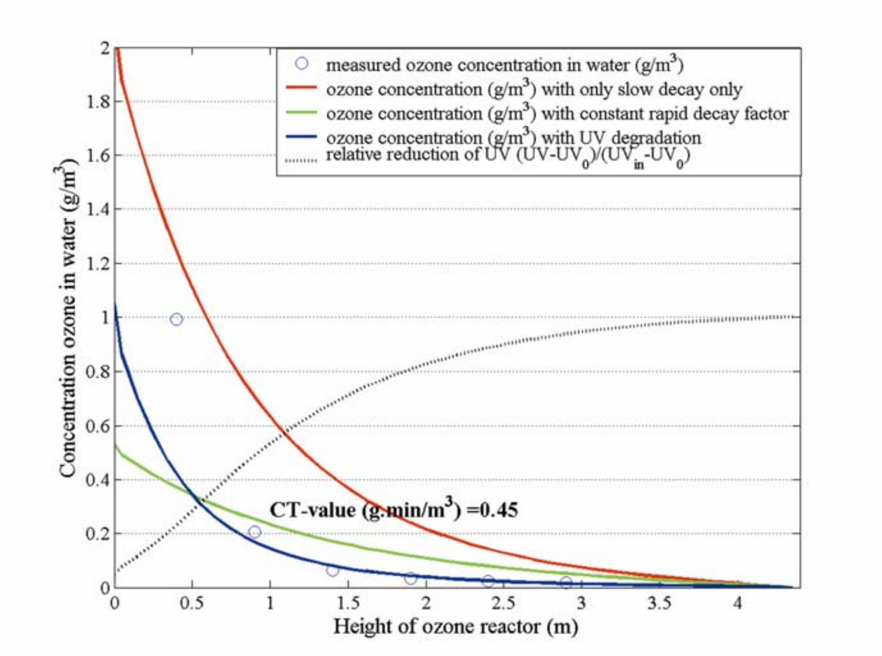

Figure 4.6 Model calibration of counter current flow and ozone dose of 3.5 g/m^3

4.4.3 Determination of CT-values in bubble and contact columns

The CT-value in the bubble and contact columns can be determined by integrating the ozone concentration profile in time. From figure 4.5 and 4.6 it can be concluded that for pilot plant Weesperkarspel, a temperature of 20°C and an ozone dose of 3.5 g/m^3, the CT-value in the co-current bubble column is 1.2 g.min/m^3 and in the counter current column is 0.45 g.min/m^3.

The CT-value in the contact columns is also determined under the same conditions (see figure 4.7). The surface area of the contact column is assumed to be twice the surface area of the bubble column. In the upper figure the CT-value after the co-current bubble column is presented, while in the lower figure the CT-value after the counter current bubble column is represented. The CT-values are 0.26 and 1.13 g.min/m^3 respectively. It can be concluded that in the system of co-current flow in the bubble column about 80% of the CT-value occurs in the bubble column. In the system with counter current flow in the bubble column this percentage is about 30% and thus not negligible. The total CT-values of both systems are not the same, mainly because the efficiency of a counter current flow system is slightly higher.

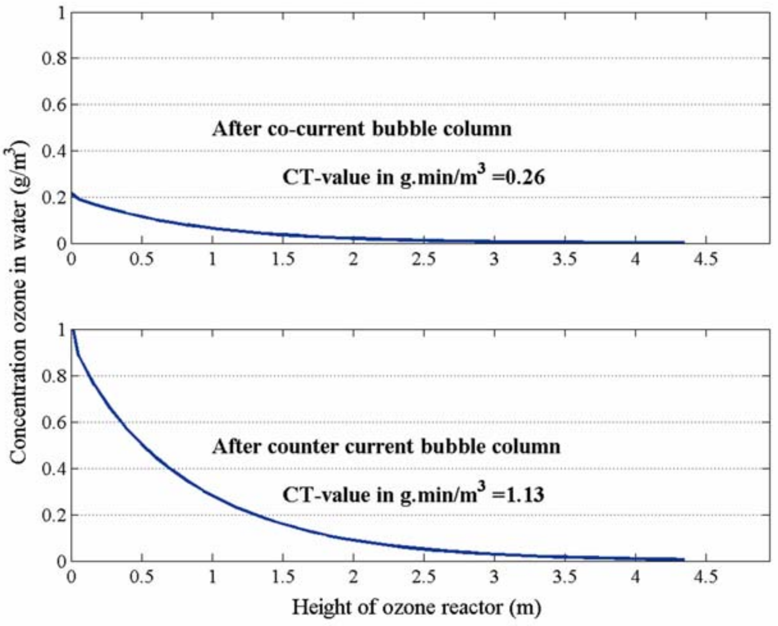

Figure 4.7 Ozone profile in contact column after co-current and counter current bubble column.

4.5 Discussion

From the modelling results it can be concluded that the rapid decay of ozone plays an important role in the prediction of the ozone profile in the bubble column. The rapid decay is not constant, but decreases in the direction of the flow in the reactor. A relation can be found between the degradation of UV absorbance and the rapid decay of ozone in water. Neglecting the rapid decay overestimates the ozone concentration in the column and considering a constant rapid decay rate gives an underestimate of the effluent ozone concentration (see figure 4.5 and 4.6).

The other processes in the reactor such as advection, dispersion, slow decay and gas transfer are fairly well understood, but still uncertainty exists about the exact values of the parameters. In the experiments on slow decay, the decay rate is influenced by the ozone dose (see figure 4.4). A reason for a lower k_{O3} value at the higher initial ozone dose is that at lower ozone doses interference occurs with the rapid decay component. This is conform the observations of Park et al. (2001). From the calibration of the model it can also be concluded that UV absorbance degradation is complete at an ozone dose in the neighbourhood of 3.5 g/m^3. In figure 4.5 and 4.6 it is shown that the relative UV absorbance in the effluent is (almost) equal to 0 and thus no further rapid decay will take place in the contact chambers.

During the measurements in the pilot plant CT-values in the bubble column are determined. With the ozone dose of 3.5 g/m^3 at a temperature of 20 ^{o}C, the CT value in the column with co-current flow is determined as 1.2 min.g/m^3. With decay rates of 0.014/s, in the contact column the CT-value is 0.26 min.g/m^3. For the counter current bubble column the values are 0.45 and 1.15 min.g/m^3 respectively. The contribution of the bubble column to the total CT-value is thus between 30 and 80% and cannot be neglected.

For the operation of the ozone reactor, the (model) prediction of the ozone profile in the bubble column is therefore of importance. Further calibration will lead to a model that can predict the ozone profile under different circumstances (temperature and UV absorbance). For incorporation of temperature in the model, adaptations must be made with respect to the kinetic parameters. It has been found that the temperature dependence of reaction rate constants can be well represented by an equation, known as Arrhenius' law:

$$k = k_0 \exp \frac{-E}{RT}$$

Where k_0 is the frequency factor representing the number of molecular collisions per time and E is the activation energy (J/mol) and R the universal gas constant (J/mol). According to this expression a semilog plot of the rate constant as a function of the inverse of the absolute temperature should be linear (Montgomery, 1985).

At the full-scale water treatment plant Weesperkarspel of Amsterdam Water Supply, ozone is dosed in 4 parallel streams by a single co-current column. The gross ozone dose is approximately 2.25 g/m^3 in winter and 1.75 g/m^3 in summer. Although decay of ozone in summer is high, the dose is lowered because of rapid clogging of the subsequent (biological) activated carbon filters. A more rational approach would be to determine the required (temperature dependent) CT-value, based on influent pathogen concentration and the required decimal elimination by ozone. With the model a prediction can be made of the ozone profile in the bubble column and the contact chambers, varying with influent UV absorbance and temperature. This procedure will lead to a minimisation of the ozone dose without deterioration of the water quality in terms of hygienic parameters and avoiding unwanted by-product formation as bromate. When rapid clogging of the filters becomes a problem, due to the proposed operation strategy, alternatives must be considered. Either the configuration of the filters must be changed or the water must be pre-treated, reducing the UV absorbance in the influent and thus managing the formation of biodegradable organic matter. The pilot plant Weesperkarspel is being automated and on-line monitoring equipment has been installed. The model will be used for model predictive control to implement the proposed operation strategy.

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5 DIMINISHING REGENERATION FREQUENCY OF GAC FOR MICRO-POLLUTANT REMOVAL

5.1 Introduction

In drinking water treatment granular activated carbon (GAC) filters are used to adsorb dissolved organic matter, both Natural Organic Matter (NOM) and micro-pollutants. The filters become saturated after a certain period (months or years) and break-through occurs. The activated carbon is then regenerated and re-used. When the influent concentration is constant the effluent concentration for a single compound is an s-shape function (break-through curve). The aim of the filters is to remove the target compound sufficiently to meet the guidelines for drinking water quality and to have a safety barrier against unknown organic micro-pollutants.

The design of an activated carbon filter is based on pilot plant research (or laboratory tests). In that phase the type of activated carbon is selected and the optimal contact time and filter bed height are determined. This research takes at least one year of experimentation with several filter columns in parallel. During the design phase the number of filters and the configuration of the filters (parallel or in series) are determined. As not all configurations can be tested in pilot plants, models can help to translate laboratory and pilot plant studies to full-scale applications.

Modelling of activated carbon filtration can have different benefits, related to design, monitoring, operational strategies and trend analysis. In the past many modelling exercises were executed to determine the design configuration of filters related to different target compounds (Crittenden et al, 1987), to translate pilot plant research to full-scale application (Clark, 1987; Summers and Roberts, 1984), to translate lab scale experiments to pilot and full scale application (Heijman et al, 2001) and to determine the remaining life of a granular activated carbon filter (Knappe et al, 1994).

After construction of the filters it is the responsibility of the operator to control the installation in such a way that the guidelines are met and regeneration is only executed when it is strictly necessary. Although the guidelines are based on risk assessments assuming long-term exposure (including safety factors), in practice regeneration of one or more filters takes place when the company guidelines of the quality parameter (sometimes stricter than the drinking water guidelines) in the product are reached. Consequently, during long periods the effluent concentrations are much lower than stated in the guidelines. Simulation of the impact of control alternatives can support the operator to make decisions on operation and determine the influence of disturbances on the effluent quality.

Manipulation of activated carbon filters are restricted to the distribution of flow over the filters, backwashing and regeneration of the filters and operation of the filters in series or in parallel (if in the design phase this option is taken into account).

The costs of operation and the impact for the environment are determined by the regeneration frequency of the filters, the energy consumptions of the pumps and the frequency of backwashing of the filters. Regeneration, however, is predominant so a reduction of the frequency of regeneration, will have a positive impact on costs and environmental impact.

Activated carbon filtration is a slow reacting process and instant changes in the influent do not have immediate effect on the quality of the effluent. In addition, frequent measurements of micro-pollutants in the effluent of individual filters is an expensive operation. Therefore, continuous evaluation of the effluent water quality cannot be carried out. With model predictions, however, the effluent of the activated carbon filters can be monitored continuously. In addition, operational scenarios can be evaluated and the best solution can be implemented. Product water quality will still be measured to check the controlled situation. With these data the model can be re-calibrated and used for the periods afterwards.

In this chapter, modelling is done using a conceptual/phenomenological, dynamic model based on kinetics and mass balance equations. The model describes GAC filtration in a pseudo moving bed configuration, where the influent of the second filter is changing due to gradual break-through of the first filter. The model is fitted on data of full-scale and pilot plants and operational strategies are evaluated. The emphasis is on the removal of organic micro-pollutants, which is influenced by the preloading of Natural Organic Matter. Based on the formulae described below, a model has been made with the Stimela platform in Matlab/Simulink (see chapter 3).

Important assumptions in this model are:

- Removal of micro-pollutants is influenced by the influent NOM concentration
- Mass transfer coefficient is dominated by internal surface diffusion processes in the carbon grains (in contrast to water-film diffusion around the grain)
- Backwashing of activated carbon filtration is not influencing the stratification of the adsorbed organic matter in the filter.

After describing the process mathematically, two different cases are evaluated. At water treatment plant (WTP) Rodenhuis (Hydron ZH) the full-scale situation is compared to previous pilot plant research. In a second case, the model is applied to WTP Reijerwaard (Hydron ZH) with higher background organic matter levels, but using the same carbon type.

Finally, the performance of filters in series is compared to parallel operation and it is calculated how an operational improvement, i.e. better distributed regenerations of individual filters in time, can reduce cost and environmental emissions, without violating the (company) guidelines.

5.2 Modelling of granular activated carbon filters

5.2.1 Transport of a compound through a reactor in water

For the removal of (micro-) pollutants from the water phase by GAC filtration, neglecting dispersion, decay and advection in the solid phase and considering the water velocity in the pores, the overall equations for transport (see chapter 2)

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u_s \frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}(c, c_s) = 0$$

are reduced to:

$$\frac{\partial c_{OM}}{\partial t} + \frac{u}{\varepsilon}\frac{\partial c_{OM}}{\partial x} + f_2(c_{OM}, c_{s,OM}) = \frac{\partial c_{OM}}{\partial t} + \frac{Q}{A_T \varepsilon}\frac{\partial c_{OM}}{\partial x} + f_2(c_{OM}, c_{s,OM}) = 0$$

$$\frac{\partial c_{s,OM}}{\partial t} + f_{2,s}(c_{OM}, c_{s,OM}) = 0$$

During the transport process (micro-) pollutants are adsorbed on the activated carbon. The amount of adsorbed (micro-) pollutants is equal to the amount of (micro-) pollutants taken out of the water (mass balance). For a stationary flow, the mass balance can be written as:

$$\left.\begin{aligned} \frac{u}{\varepsilon}\frac{\partial c_{OM}}{\partial x} &= -f_2(c_{OM}, c_{s,OM}) \\ \frac{\partial c_{s,OM}}{\partial t} &= f_{2,s}(c_{OM}, c_{s,OM}) = -u\frac{\partial c_{OM}}{\partial x} \end{aligned}\right\} \Rightarrow f_{2,s}(c_{OM}, c_{s,OM}) = \varepsilon\, f_2(c_{OM}, c_{s,OM})$$

The concentration of the compound in the solid phase is given as mass per volume reactor, whereas water flows with pore velocity u/ε (m/s). The transfer rate to the solid phase is therefore different from the transfer rate from the water. The difference is calculated by multiplication with the porosity ε (-).

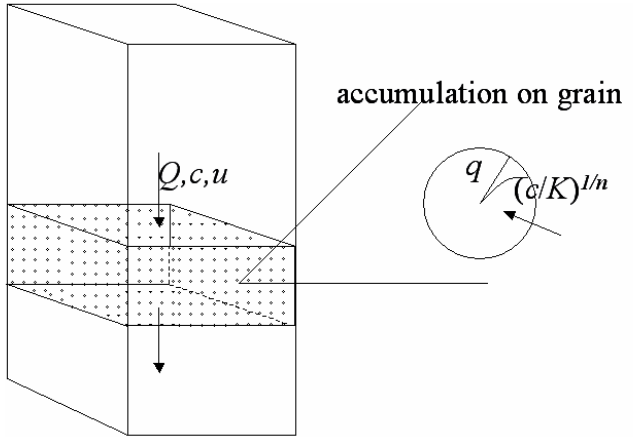


Figure 5.1 Impression of activated carbon filter

It is now necessary to find a relation for the transfer component (f_2) of the equations.

Where

Q	water flow (m^3/s)
u	superficial water velocity (m/s)
A_T	total surface area of reactor (m^2)
ε	porosity (-)
c_{OM}	concentration of micro-pollutant in water (g/m^3)
$c_{g,OM}$	concentration of micro-pollutant on carbon grains (g/m^3)

5.2.2 Transfer of micro-pollutants from water phase to carbon grains

The adsorption capacity (q_{max} in mg/kg) is determined empirically for different concentrations in water (or water to carbon ratios). When the results are plotted on logarithmic scale a straight line is found for the relation between the water concentration and the adsorption capacity. This relation can be written by the Freundlich isotherm (Sontheimer, 1988):

$$q_{\max} = K c_e^{1/n}$$

Where

K	Freundlich constant ($(g/kg)(g/m^3)^n$)
$1/n$	Freundlich constant (-)
c_e	equilibrium concentration (g/m^3)

The kinetics of adsorption consists of two basic steps: mass transfer from the water phase to the solid phase and intra-particle transport. Mass transfer of (micro-) pollutants to the solid phase is controlled by the laminar water film (film diffusion). Transport of (micro-) pollutants in the particle can be described by two mechanisms: pore diffusion and surface diffusion. Normally the intra-particle diffusion is predominant and film diffusion is neglected. Maximum loading of the filters is reached when equilibrium between the concentration of (micro-) pollutants in the water phase and on the solid phase occurs.

A number of complex mathematical models are developed to describe the adsorption process in the activated carbon filters (Crittenden et al., 1978, Hand et al, 1984). Simplified models are mainly useful to model activated carbon filtration in full-scale plants. Examples of these models are the "general logistic function" (Clark, 1987) and the use of the "linear driving force" assumption for surface diffusion to describe intra-particle mass transfer, neglecting water film diffusion (Peel and Benedek, 1981, Heijman, 2002). The last simplification is further used in this study.

The intra-particle mass flux for surface-diffusion is described by Sontheimer et al. (1988).

$$\phi_s = D_s \rho_p \left(\frac{dq}{dr} \right)$$

The mass balance for a carbon particle, calculating the average carbon loading over the particle:

$$V_p \rho_p \frac{\partial \bar{q}}{\partial t} = A_p D_s \rho_p \left(\frac{\partial q}{\partial r} \right)_{r=\frac{d_p}{2}}$$

The surface diffusion at the surface of the carbon grain is approximated by a linearisation of the loading at the surface of the carbon grain and the average loading over the complete grain (Sontheimer, 1988).

$$D_s \left(\frac{\partial q}{\partial r} \right)_{r=\frac{d_p}{2}} = \beta_s \left(q_{r=\frac{d_p}{2}} - \bar{q} \right)$$

This turns into:

$$\frac{d\bar{q}}{dt} = \frac{6}{d_p} \beta_s \left(q_{r=\frac{d_p}{2}} - \bar{q} \right)$$

Substituting:

$$q_{r=\frac{d_p}{2}} = Kc^{1/n}$$

Resulting in the differential equation for internal mass transport:

$$\frac{d\bar{q}}{dt} = \frac{6}{d_p}\beta_s\left(Kc^{1/n} - \bar{q}\right)$$

Where

φ_s	mass flux into carbon grains (g/m^2.s)
ρ_p	density of carbon grain (kg/m^3)
D_s	surface diffusion coefficient (m^2/s)
q	loading of carbon grain (g/kg)
V_p	volume of particle (m^3)
A_p	surface area of particle (m^2)
d_p	diameter of carbon grain (m)
r	radius (m)
β_s	surface diffusion transfer coefficient (m/s)

5.2.3 General equations for transport and adsorption to activated carbon

The equations for adsorption, neglecting dispersion and decay of the compound, become:

$$\frac{\partial c_{OM}}{\partial t} = -\frac{u}{\varepsilon}\frac{\partial c_{OM}}{\partial x} - \frac{\rho}{\varepsilon}\frac{\partial q_{OM}}{\partial t} = -\frac{u}{\varepsilon}\frac{\partial c_{OM}}{\partial x} - \frac{\rho}{\varepsilon}\frac{6}{d_p}\beta_s(Kc_{OM}^{1/n} - \overline{q_{OM}}) = -\frac{Q}{A_T\varepsilon}\frac{\partial c_{OM}}{\partial x} - k_2(Kc_{OM}^{1/n} - \overline{q_{OM}})$$

$$\frac{\partial \overline{q_{OM}}}{\partial t} = -\frac{u}{\rho_p}\frac{\partial c_{OM}}{\partial x} = \frac{Q}{A_T\rho_p}\frac{\partial c_{OM}}{\partial x}$$

K en β_s values are largely dependent on the type of organic matter that must be adsorbed, the preloading on the activated carbon and the type of carbon (see next section), while *1/n* is in the range of 0-1. The density of the carbon is normally between 400 and 600 kg/m^3.

At the beginning of the run time, the loading of the carbon is zero and the mass transfer rate is at its maximum. The higher the loading is, the smaller the mass transfer rate until equilibrium. The higher the influent concentration is, the higher the loading capacity of the filter and the higher the driving force. The adsorption rate is thus determined by the influent concentration, the loading of the carbon and the mass transfer coefficient. The mass transfer coefficient is determined by the nature of the (micro-) pollutants, the type of carbon and some water quality parameters, where background organic matter is most predominant. When after a long period of high influent concentrations the influent concentration decreases desorption can occur (reversible adsorption).

5.2.4 NOM influencing adsorption of micro-pollutants

Compounds that adsorb easily have a high value of Freundlich *K*.
The value of *K* increases in the following cases:

- Increase in molecular weight
- Substitution with halogens
- Increase in the number of double bounds

The adsorption of different organic compounds varies largely. The value of *K* decreases in case of substitution with polar groups such as COOH and OH. Pesticides which are polar will be removed less than pesticides which are a-polar. When several organic compounds are present in the water, adsorption of compounds with the highest *K*-value is predominant. The content of natural organic matter (NOM) 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 (Weber, 2002). Adsorption capacity of micro-pollutants decreases with preloading time. Preloading by NOM also leads to decreased adsorption kinetics as indicated by the surface diffusion coefficients (Knappe, 1994). The adsorption capacity of micro-pollutants, for example atrazin, is strongly hindered for DOC levels above 3 g/m^3, where the characteristics of DOC play also an important role (Bernazeau et al., 1994).

5.3 Materials and methods

5.3.1 Modelling approach

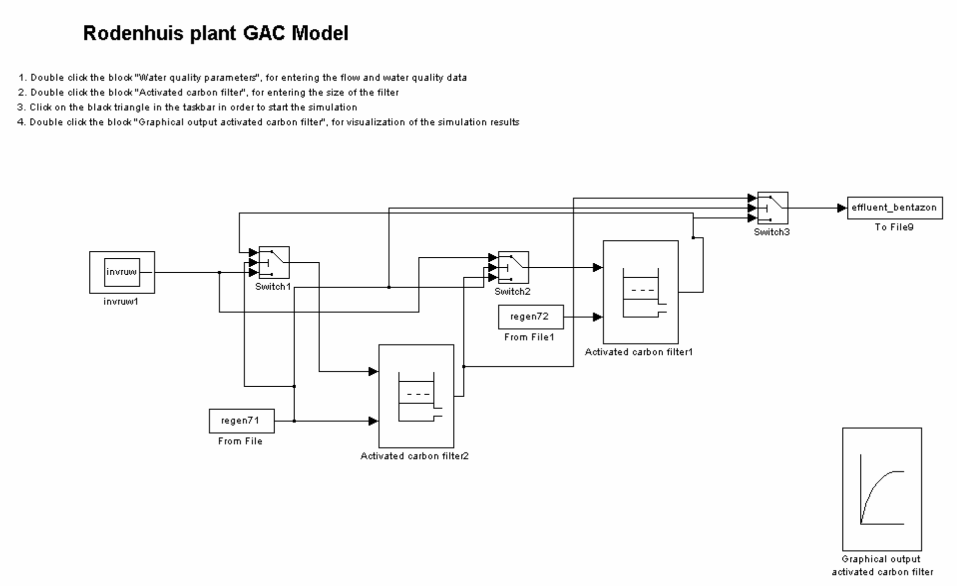
The model is developed within the Stimela environment (see chapter 3).

The model consists of:

- Input disturbance variables:
    - water flow Q (m^3/s)
    - bentazon concentration c_{OM} (g/m^3)
- Input manipulated variables:
    - run time (s)
    - order of filters
- State variables:
    - bentazon concentration c_{OM} (g/m^3)
    - loading of filter bed q_{OM} (g/kg)

- Output water quality variables:
    - water flow Q (m^3/s)
    - bentazon concentration c_{OM} (g/m^3)
- Extra output variables:
    - bentazon concentration over the height of the reactor (g/m^3)
    - loading of filterbed over the height of the reactor (g/kg)
- Physical parameters:
    - surface area of reactor A_T (m^2)
    - filter bed height L_b (m)
    - filter bed porosity ε (-)
    - diameter of carbon grain d_p (m)
- Calibration parameters
    - transfer coefficient k_L (m/s)
    - Freundlich constant K (g/kg)(g/m^3)^n
    - Freundlich constant $1/n$ (-)
    - number of unit elements (-)

At start-up of the reactor (initial condition) the bentazon concentration in the filter is equal to the input concentration and the loading of the activated carbon is absent.



Rodenhuis plant GAC Model

1. Double click the block "Water quality parameters", for entering the flow and water quality data
2. Double click the block "Activated carbon filter", for entering the size of the filter
3. Click on the black triangle in the taskbar in order to start the simulation
4. Double click the block "Graphical output activated carbon filter", for visualization of the simulation results

Figure 5.2 Representation of Stimela model for activated carbon filter in pseudo moving bed configuration

5.3.2 Description of WTP and pilot plant Rodenhuis

Since 1993 activated carbon filtration is being applied at water treatment plant (WTP) Rodenhuis of Hydron ZH for the removal of bentazon, which originates from the river Lek. The Lek water infiltrates in the riverbank and is abstracted to act as the source for drinking water. The treatment plant consists of aeration, filtration, aeration, rapid sand filtration and activated carbon filtration. In 1993 pilot research was executed to determine the type of activated carbon to be applied at WTP Rodenhuis. Chemviron F400 was selected because it has the longest run times until break-through (0.1 10^{-3} g/m^3 in the filtrate) and the highest cumulative loading (Beerendonk, 1994). The specification of the pilot plant is given by:

- Average flow	1590 m^3/s
- Filter surface	0.04909 m^2
- Filter bed height	1.5 m
- Contact time (EBCT)	600 s
- Carbon type	Chemviron F400

The breakthrough curves at different heights in the filter filled with Chemviron F400 are shown in figure 5.3.

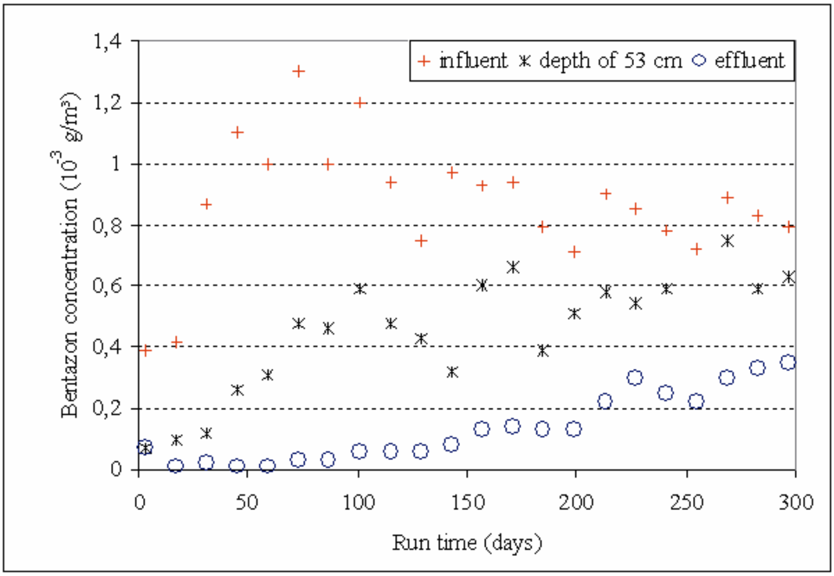


Figure 5.3 Break-through of bentazon in pilot plant Rodenhuis

At WTP Rodenhuis two filter buildings with 4 double filter sets are installed. These filter sets act in a tandem as a pseudo moving bed system. Some specifications are given below:

Average flow	576 10^4 m^3/s
Number of filters	2 buildings with 2x4 filters per building
Filter surface	27 m^2
Filter bed height	1.6 m
Contact time (EBCT)	2x780 s
Carbon type	Chemviron F400

At the end of a run-time, the carbon of the first filter is regenerated. The raw water inflow is then connected to the second filter and the effluent flows into the regenerated first filter.

At the time of start-up of the activated carbon filters in 1993, only the first 8 filters were filled and taken in production. In 1994 the second filters were taken into operation. In figure 5.4 the bentazon concentration in the clear water (in two sampling points) of the full-scale plant is shown. From the figure the start-up of activated carbon in 1993 is evident.

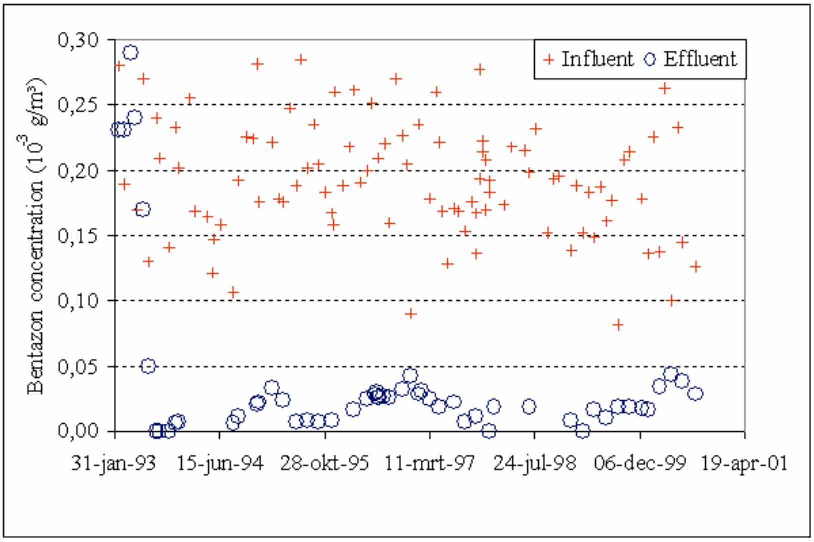


Figure 5.4 Bentazon in the raw and product water of WTP Rodenhuis

In the beginning of 1995 the bentazon concentration in the clear water was increasing relatively rapidly, because all filters were simultaneously taken into operation and thus break-through occurred at the same time. In the first half of 1995 8 filters were regenerated. The same phenomenon took place at the end of 1996, which resulted in the regeneration of 5 filters in the second half of 1996 and another 7 in 1997. In 1998 5 regenerations were executed and the bentazon concentration was kept far under the company guideline of 0.05 10^{-3} g/m^3, as can be observed in figure 5.4. In 1999 4 regenerations were realised. It is expected that after 2000 the number of regenerations will be 5 per year. The DOC levels at WTP Rodenhuis are in the range of 2.2 g/m^3.

Figure 5.5 WTP Reijerwaard, Hydron ZH

5.3.3 Description of WTP Reijerwaard

Like WTP Rodenhuis, WTP Reijerwaard also treats riverbank groundwater with a pseudo-moving-bed principle. At Reijerwaard two sets of two filters are installed. The influent concentrations of bentazon are similar to the concentrations at WTP Rodenhuis (see figure 5.6) and the same carbon type is used. DOC levels, however, are considerably higher: DOC=4.9 g/m^3.

Some specifications are given below:

Average flow	108 10^4 m^3/h
Number of filters	2x2 filters
Filter surface	26.3 m^2
Filter bed height	2 m
Contact time (EBCT)	2x1200 s
Carbon type	Chemviron F400

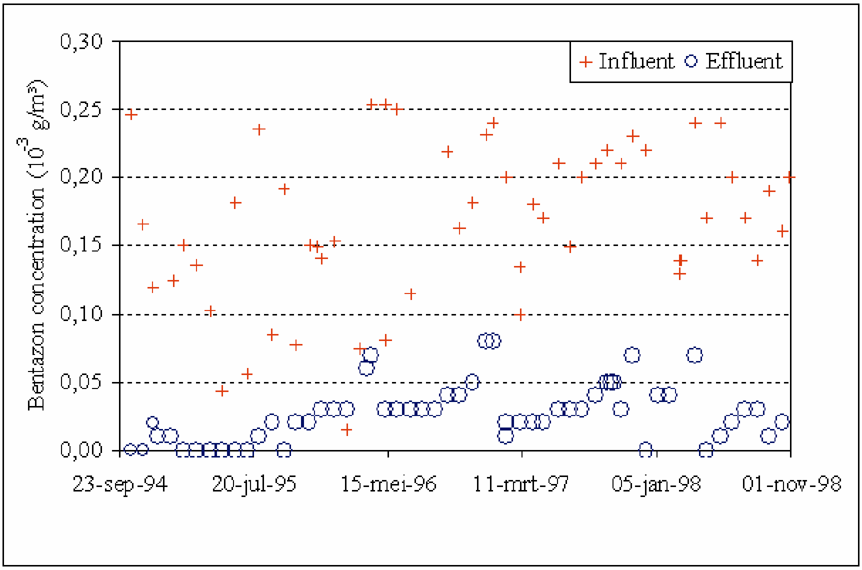


Figure 5.6 Bentazon in the raw and product water of WTP Reijerwaard

5.4 Application of model to WTP Rodenhuis and Reijerwaard

5.4.1 Calibration of model parameters

For calibration of the model the k_2-, K- en n-values of the partial differential equations must be determined. K- and n-values can be determined from data of full-scale and pilot plant, if total breakthrough occurs in the filters. In this case, the maximum loading capacity is determined based on accumulation of pollutants in the filter and mass transfer coefficient k_2 no longer plays a role.

If total break-through is not observed, extrapolation of existing data is necessary. Extrapolation is based on the fact that breakthrough behaves as an s-curve. Plotting the s-curve on log-log scale it becomes a straight line, which can be easily extrapolated. For WTP Rodenhuis total breakthrough does not occur and for different filters the loading capacity is determined. For an example of the determination of the loading capacity of one of the filters of WTP Rodenhuis see figure 5.7. The average loading capacity of all filters is 34 10^{-3} g/kg with an average influent quality of 0.215 10^{-3} g/m^3 bentazon.

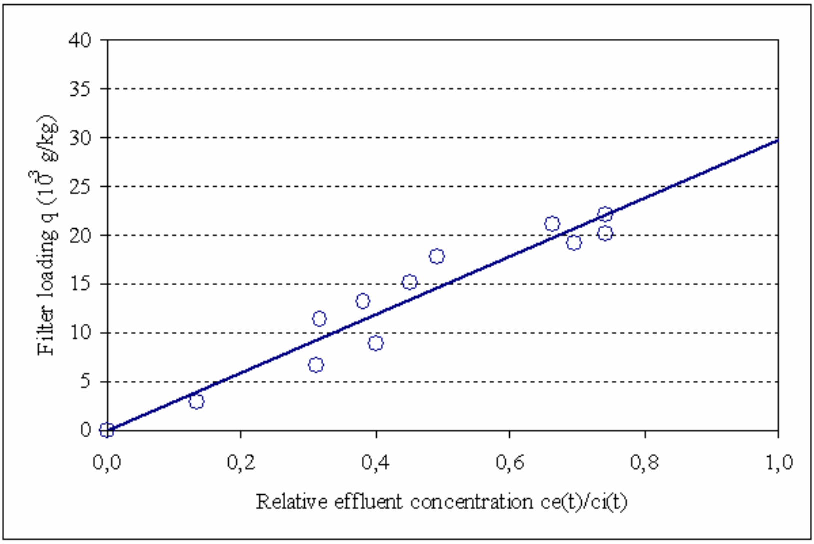


Figure 5.7 Determination of loading capacity of filter 72 of WTP Rodenhuis (q_{max}=30 10^{-3} g/kg)

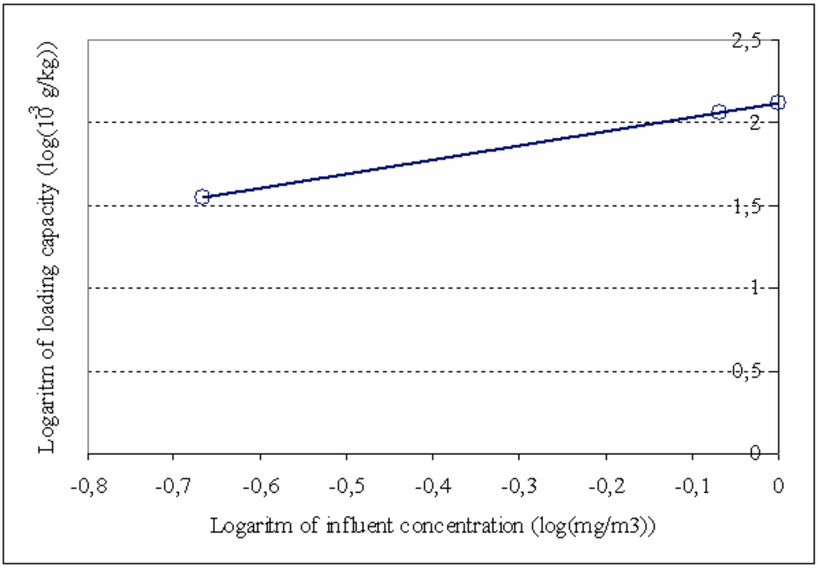


Figure 5.8 Freundlich isotherm determined by data from pilot plant and WTP Rodenhuis

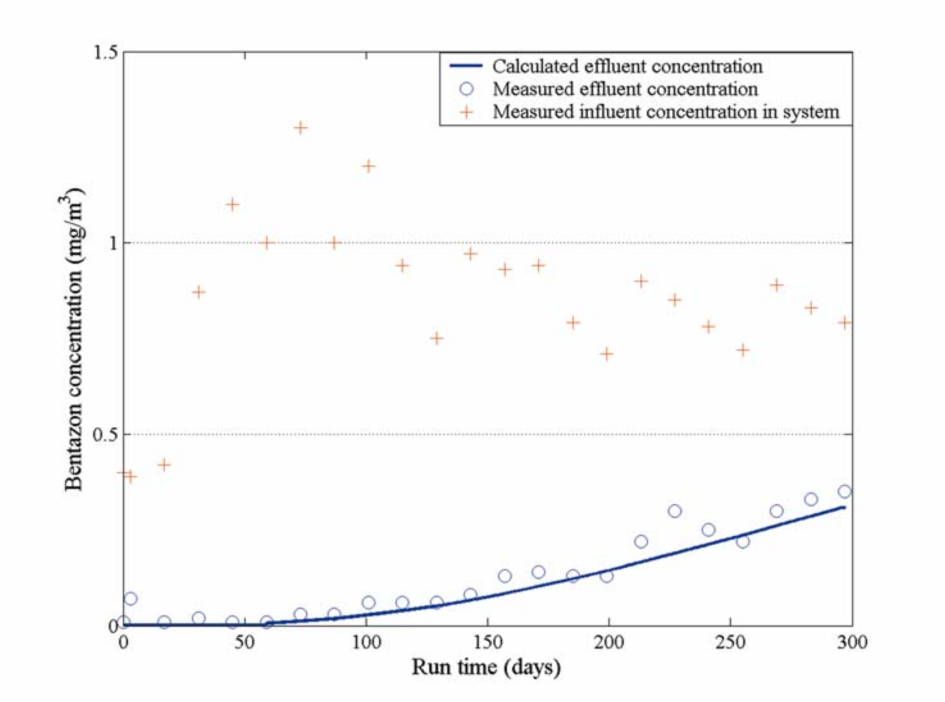


Figure 5.9 Influent and effluent bentazon concentration (measured and calculated) of pilot plant Rodenhuis

As can be observed from figure 5.3 and 5.4, the influent concentrations during pilot plant research are considerably higher than the influent concentrations of bentazon during full-scale operation. The loading capacity of the carbon in the pilot plant is determined directly through the saturation of the top layer (at 53 cm depth) of the pilot filter and is 115 10^{-3} g/kg with an average influent quality of 0.85 10^{-3} g/m^3 bentazon. From these two points the *K*- and *1/n*-value can be determined as 133 (mg/kg) (mg/m^3)^n= 4.72 10^{-5} (g/kg) (g/m^3)^n and 0.87 respectively (see figure 5.8).

k_2-value is then determined by fitting the model to the pilot plant effluent data (see figure 5.9).

5.4.2 Model validation of the full-scale WTP Rodenhuis

With the dynamic model the activated carbon filters of WTP Rodenhuis (8 sets of two filters in series in pseudo moving bed configuration) are simulated under changing influent concentrations. The calibration parameters determined in the preceding section are used for simulation of WTP Rodenhuis. From figure 5.10 and 5.11 (example of filter 71 and 72) it can be concluded that the simulation describes the measurements fairly well. The measured effluent bentazon data, however, are unstable. This can be due to sampling problems, short-circuiting, disturbances in the filter bed after backwashing or variation in the flow (assumed to be constant). In addition, the errors in the calculation of the first filter propagate to the second filter. Therefore, the break-through of filter 71 in the start-up phase is more prominent than supposed and so filter 72 receives more bentazon than expected. The preloading of filter 72 with bentazon is higher in reality and so the model predicts lower effluent concentrations in the second period after regeneration of filter 71.

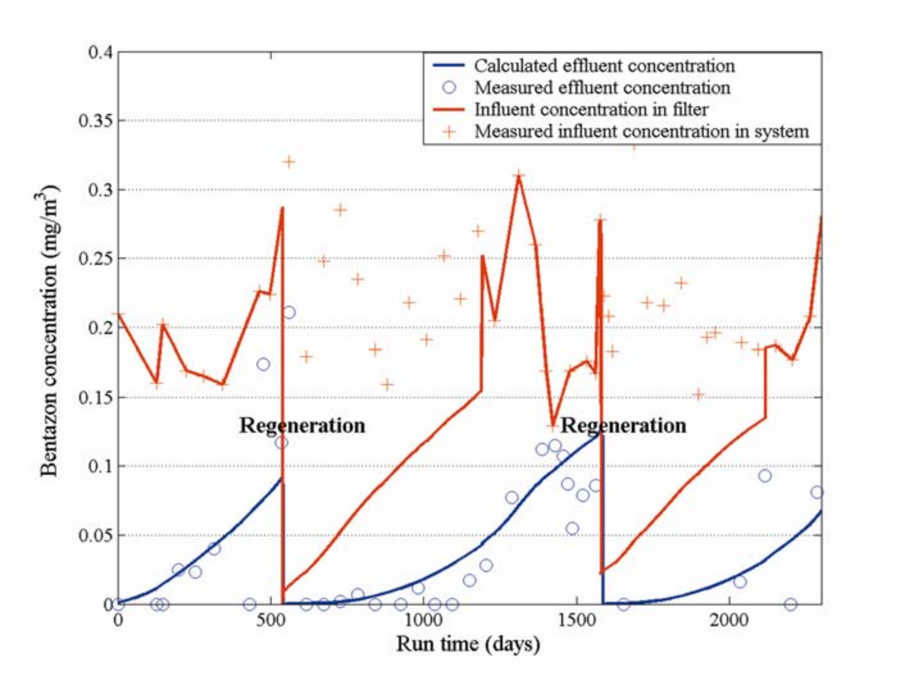


Figure 5.10 Influent and effluent bentazon concentration of filter 71 of WTP Rodenhuis

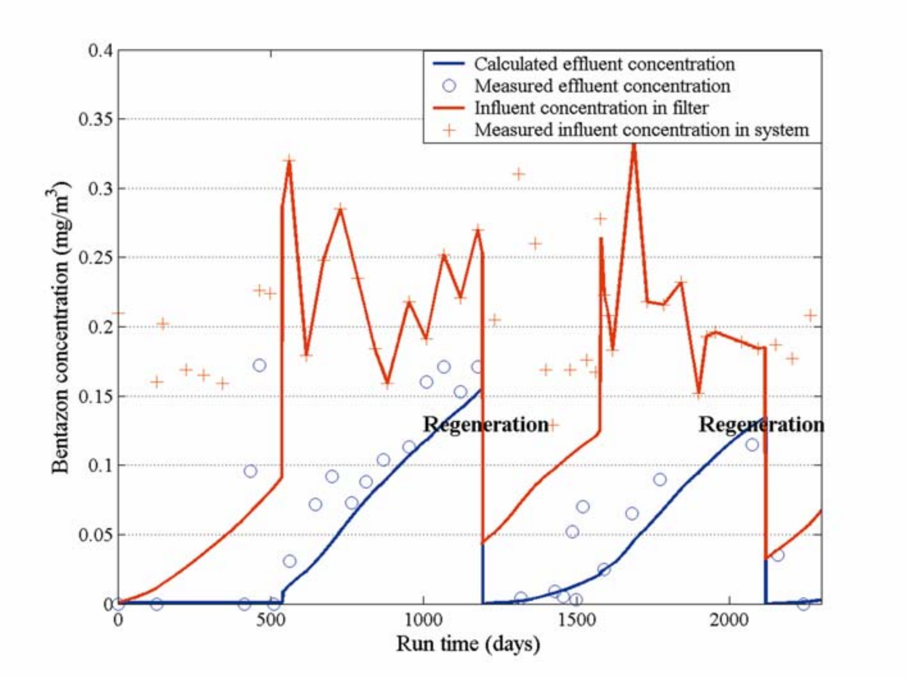


Figure 5.11 Influent and effluent bentazon concentration of filter 72 of WTP Rodenhuis

5.4.3 Application of calibrated model for WTP Reijerwaard

At WTP Reijerwaard the background organic matter levels are considerably higher than at WTP Rodenhuis: DOC = 4.9 g/m^3 (compared to 2.2 g/m^3 at WTP Rodenhuis). That is why the calibration parameters used for the modelling of WTP Rodenhuis can not directly be applied for the simulation of WTP Reijerwaard. The maximum loading capacity of bentazon will be lower at WTP Reijerwaard compared to WTP Rodenhuis. This is expressed by a lower Freundlich *K*-value. The kinetic constant and the Freundlich *1/n*-value are assumed to be unchanged. For atrazine a reduction of the Freundlich *K*-value with a factor 2.4 was found when DOC levels where increased from 2.2 to 4.9 g/m^3 (Bernazeau et al., 1994). The same reduction is applied for WTP Reijerwaard and consequently the Freundlich *K*-value becomes 55 (mg/kg) (mg/m^3)^n=1.97 10^{-5} (g/kg) (g/m^3)^n.

From figure 5.12 and 5.13 it can be concluded that the model, under prevailing assumptions, predicts fairly well the effluent bentazon concentrations.

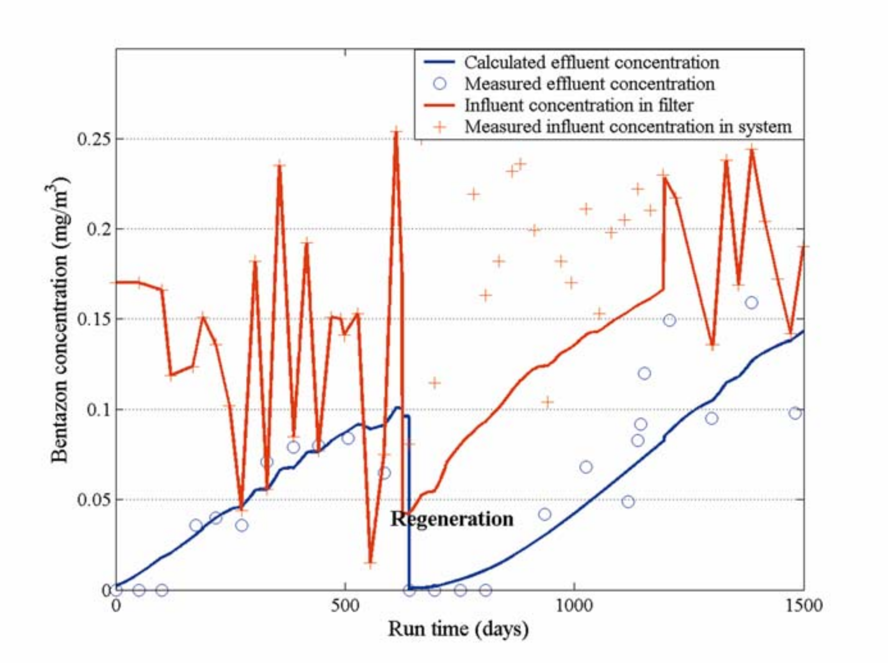


Figure 5.12 Influent and effluent bentazon concentration of filter 1 at WTP Reijerwaard

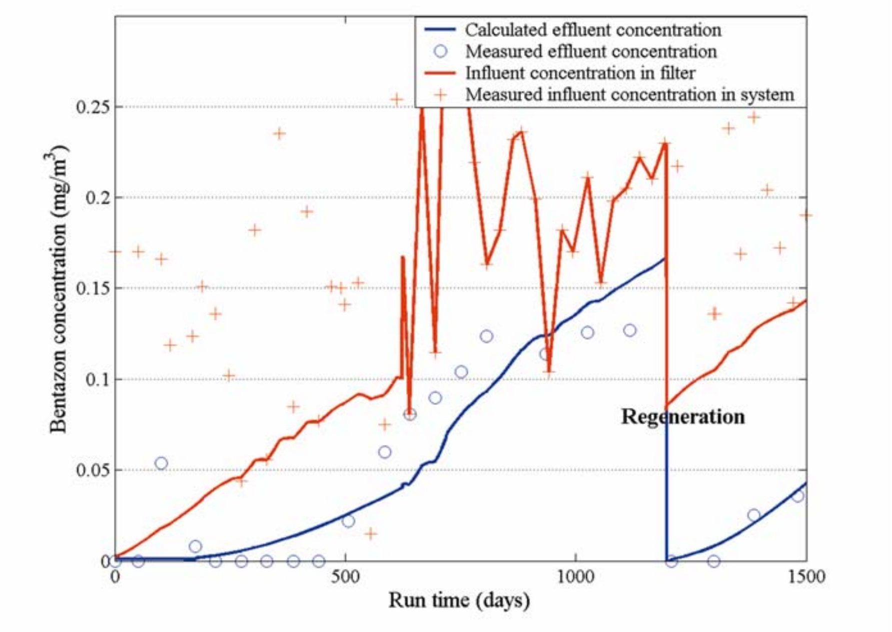


Figure 5.13 Influent and effluent bentazon concentration of filter 2 at WTP Reijerwaard

5.5 Model supported operation improvements

With the model different alternative solutions for operation are evaluated. At WTP Reijerwaard the effects of abandoning the pseudo-moving bed configuration had to be determined, because the future hydraulic capacity of the filters would be too low to operate the filters in series. A quality and cost comparison was made to evaluate the impact of parallel operation of the filters. In figure 5.14 the difference between the product water quality of a plant operated in pseudo moving bed configuration and a plant operated with parallel connected filters is shown.

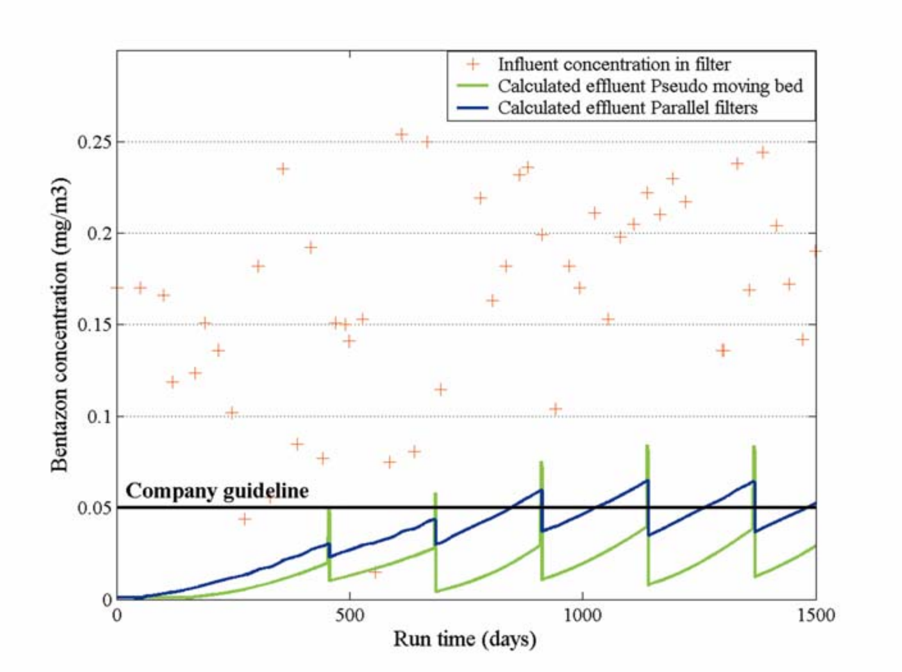


Figure 5.14 Difference between pseudo moving bed configuration and parallel filter at WTP Reijerwaard (run time of filter = 2.5 years)

It was concluded from the modelling exercise that under the actual circumstances, with a maximum concentration of 0.05 mg/m^3 bentazon in the product water, regeneration would be 20% more frequent under parallel conditions (once every two years instead of once every 2.5 years), which would result in an increase of regeneration costs of about € 6000,- per year. During one and a half year of experimentation at WTP Reijerwaard the parallel configuration was compared to the pseudo moving bed configuration and the model predictions of regeneration times were confirmed. During the tests positive side effects were noticed related to filter head loss. The parallel operated filters suffered a lower filter resistance and head loss build up, consequently backwashing could be less frequent.

At WTP Rodenhuis a different regeneration scheme of the activated carbon filters was determined for diminishing the costs of operation and environmental emissions (due to regeneration of activated carbon). The constraint is that the effluent water quality would never be above the company guideline of 0.05 mg/m^3, which is half of the national standard for bentazon. For individual filter sets this means that an effluent concentration of 0.1 10^{-3} g/m^3 could be tolerated. From figure 5.4, it can be observed that in practice the product concentration is far below the value that is stated in the company guidelines.

With the Stimela model the product water of 4 sets of the filters of WTP Rodenhuis is simulated, assuming a filter run time of 4 years and an equal distribution of regenerations of individual filters in time. In figure 5.15 the results are represented.

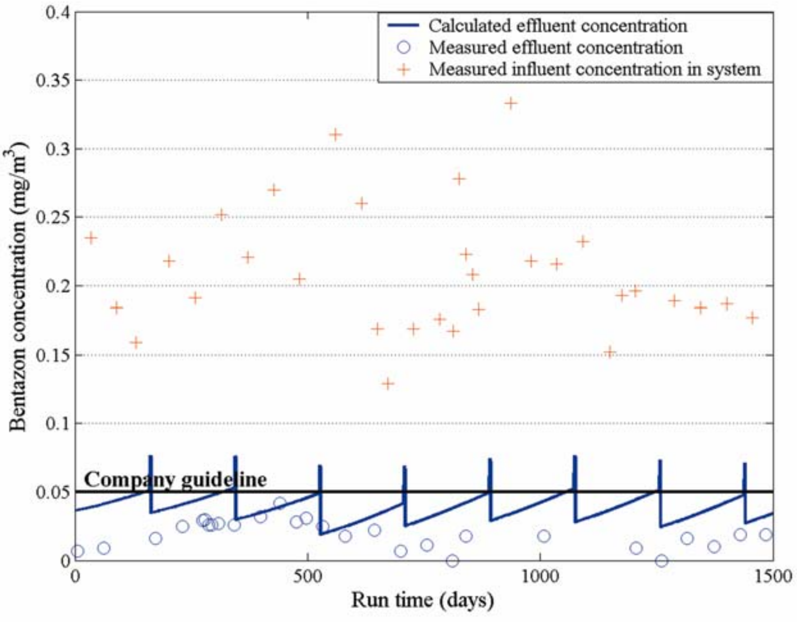


Figure 5.15 Prolonged filter run time by equal distribution of regenerations of filters at WTP Rodenhuis

When the objective of operation is to have the company guidelines as a set point, a reduction of 20% (4 generations per year instead of 5) can be reached in regeneration costs. For WTP Rodenhuis this means € 15.000,- per year.

5.6 Discussion

From this study it can be concluded that a phenomenological model can be successfully used to evaluate the performance and operation of full-scale activated carbon filters for bentazon removal. The calibrated model could also be used for similar treatment plants, facing similar problems.

Freundlich constants were derived from both pilot research and a full-scale application at the same location. The loading capacity of the activated carbon was measured directly from the top layer of the pilot plant and was determined by extrapolation from the full-scale data. The kinetic constant was determined from calibration on pilot plant data (Rodenhuis). It was assumed that the Freundlich constants were time independent and Freundlich *K*-value was only dependent on influent NOM levels. The same dependency as observed for atrazine (Bernazeau et al. 1994) was used for bentazon and this resulted in an acceptable simulation of the full-scale plant of WTP Reijerwaard. The kinetic constant for bentazon removal was not changed during the filtration process and was assumed to be independent of NOM, in contrast to what was suggested by Knappe et al. (1994).

From the evaluated scenarios it can be concluded that pseudo moving bed configurations will, in terms of effluent bentazon quality, be preferable to parallel operation. With the same number of regenerations, the average effluent quality will be lower than the mixed average effluent quality of the parallel operated filters. However, from literature it is known that parallel filters can cope economically with raw water with concentration less that 3 times the effluent quality standard (Crittenden and Weber, 1978). This is confirmed for the case of WTP Reijerwaard. Only a slight increase in regeneration costs will avoid further expansions of the treatment works. Parallel operation has additional advantages in terms of manipulations, backwashing and filter head loss.

Cost and environmental emission reductions in the regeneration of activated carbon can be reached when the effluent quality can be maintained constant on the reference value (set-point). Compared to the case of WTP Rodenhuis (figure 5.15), further prolongation of the filter run time can even be reached when declining rate filtration is applied, increasing the flow over clean filters and diminishing the flow over saturated filters. From an economic perspective modelling can help to save regeneration costs without exceeding the guidelines and standards. However, from a qualitative point of view, frequent regeneration will lead to a better product quality.

It is obvious, comparing the cases of WTP Rodenhuis and Reijerwaard, that adsorption of organic matter influences the adsorption of micro-pollutants. When the concentration of NOM can be reduced by pre-treatment or biological degradation inside the filter, better adsorption results are obtained.

With the results different design and operational scenarios can be evaluated. Especially, the start-up of a filter system and the transitions from one operation situation to another have to be managed well and the model can be useful in this respect. The model can also give better insight into the development of the product water quality, in relation to the influent flow and water quality.

GAC is a slow reacting process. The description of the dynamics enables the study of variations in flow and influent water quality, as well as the pseudo moving bed configuration. Data obtained from practice can be used for calibration without additional laboratory work.

As can be observed from the full-scale data the measurements of bentazon are rather unstable and model simulations are good tools to judge the laboratory data. In the case of WTP Rodenhuis and Reijerwaard the flows and influent concentrations are rather constant, but in case water is taken directly from the river this can be totally different and the modelling tool thus even more important. The modelling tool can be used to judge the effluent quality, without actual laboratory measurements and extreme situations can be evaluated for their risks for public health. Use of modelling of activated carbon filtration thus increases the feeling of safety and can finally lead to less analyses costs during operation and more efficient testing during design.

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6 OPTIMAL OPERATION OF PELLET SOFTENING PROCESS

6.1 Introduction

In the Netherlands central softening of drinking water is carried out mainly with pellet reactors. The pellet reactor consists of a cylindrical vessel that is partly filled with seeding material. The diameter of the seeding grain is small, between 0.2 and 0.4 mm and consequently the crystallisation surface is large. The water is pumped through the reactor in an upward direction at high velocities, maintaining the seeding material in a fluidised condition. In the bottom of the reactor chemicals are dosed (caustic soda, soda ash or lime). Calcium carbonate then becomes super-saturated and crystallises on the seeding material, resulting in the formation of pellets. At regular intervals pellets at the bottom of the reactor are removed. These pellets can be re-used in industry (Graveland et al., 1983, Van Dijk and Wilms, 1991).

Figure 6.1 Pellet softening reactor

The crystallisation process is dependent on temperature, influent water quality and dosing of chemicals. During low temperatures, the reaction rate is slow and crystallisation occurs higher in the reactor.

Softening in a reactor is normally deeper than the required levels. Therefore, part of the water can be by-passed and mixed with the effluent of the reactors. In general different reactors are installed to increase the reliability of the system and the flexibility in operation. In case of flow changes, reactors can be switched on and off, maintaining water velocities between 60 and 100 m/h.

The mixture of the effluent of the reactors and the by-pass water must be chemically stable to avoid crystallisation in the filters after the softening step. To determine optimal operation of pellet softening reactors using caustic soda (NaOH), a model has been developed. The purpose of modelling is to simulate the softening process, in order to make decisions on operation, leading finally to model predictive control of the process. During operation, water quality and flow change frequently and also manipulation of the process has influence on its behaviour. For simulation, therefore, the dynamics of the process are taken into account.

In this chapter the model is explained, validation to the case of drinking water treatment plant (WTP) Weesperkarspel of Amsterdam Water Supply and scenario calculations for optimal operation are carried out.

6.2 Modelling of pellet softening

In a softening reactor different processes occur. The water is transported through the reactor, dissolved compounds are transferred from the water to the solid phase (pellets), and the pellets grow and are transported through the reactor. The different processes in a pellet softening reactor are described below.

6.2.1 Transport of calcium ions through a pellet reactor

For the removal of calcium ions from the water by pellet softening, neglecting dispersion and decay and considering the water velocity in the pores, the overall equations for transport

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u\frac{\partial c}{\partial x} + f_1(c) + f_2(c, c_s) = 0$$

$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u_s\frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}(c, c_s) = 0$$

are reduced to:

$$\frac{\partial c_{Ca}}{\partial t} + \frac{u}{\varepsilon_e}\frac{\partial c_{Ca}}{\partial x} + f_2(c_{Ca}, c_{CaCO3}) = \frac{\partial c_{Ca}}{\partial t} + \frac{Q}{A_T \varepsilon_e}\frac{\partial c_{Ca}}{\partial x} + f_2(c_{Ca}, c_{CaCO3}) = 0$$

$$\frac{\partial c_{CaCO3}}{\partial t} + u_s\frac{\partial c_{CaCO3}}{\partial x} + f_{2,s}(c_{Ca}, c_{CaCO3}) = \frac{\partial c_{CaCO3}}{\partial t} + \frac{Q_s}{A_T}\frac{\partial c_{CaCO3}}{\partial x} + f_{2,s}(c_{Ca}, c_{CaCO3}) = 0$$

During the transport process calcium crystallises on the pellets. For a stationary flow, the mass balance can be written as:

$$\left.\begin{aligned} &\frac{u}{\varepsilon_e}\frac{\partial c_{Ca}}{\partial x} = -f_2(c_{Ca}, c_{CaCO3}) \\ &\frac{\partial c_{CaCO3}}{\partial t} + u_s\frac{\partial c_{CaCO3}}{\partial x} = -f_{2,s}(c_{Ca}, c_{CaCO3}) = -u\frac{\partial c_{Ca}}{\partial x} \end{aligned}\right\} \Rightarrow f_{2,s}(c_{Ca}, c_{CaCO3}) = -\varepsilon_e f_2(c_{Ca}, c_{CaCO3})$$

Where

A_T	total surface area of reactor (m^2)
c_{Ca}	concentration of calcium in water (mol/m^3)
c_{CO3}	concentration of carbonate in water (mol/m^3)
ε_e	porosity of expanded bed (-)
Q	water flow (m^3/s)
Q_s	pellet flow (m^3/s)
u	superficial water velocity (m/s)

The concentration of calcium in the solid phase (c_{CaCO3}) is given in mol per volume reactor. The concentration of calcium in water (c_{Ca}) is given in mol per volume water. The water flows with pore velocity u/ε_e (m/s) and, therefore, the transfer rate to the solid phase is different from the transfer rate from the water. The difference is calculated by multiplication with the porosity ε_e (-).

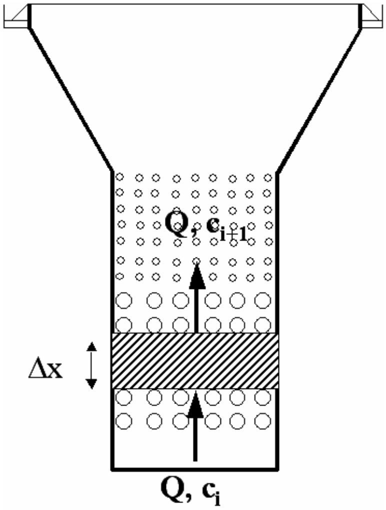

Figure 6.2 Schematic representation of pellet reactor

After starting the softening process the pellet size increases. At steady state pellet size is constant, varying over the height of the reactor, as pellet growth is neutralised by the discharge of pellets. The amount of discharged calcium ions must be the same as the amount removed during the process.

Below the transfer of the calcium ions from the water to the pellets is described. In addition, the characteristics of the fluidised bed are given in order to determine the height of the expanded bed, the porosity and the specific surface area for crystallisation.

6.2.2 Transfer of calcium ions from water to pellets

Crystallisation of calcium carbonate ($CaCO_3$) occurs via nucleation and growth. In a pellet reactor growth on the pellets is the dominant process, which is referred to as heterogeneous nucleation (Van Dijk and Wilms, 1991). Experimentally, it was found that the kinetics of heterogeneous nucleation of $CaCO_3$, can be represented by the following equation (Wiechers et al., 1975):

$$\frac{dc_{Ca}}{dt} = -k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$

Where

k_T	kinetic constant (m^4/mol.s)
a	specific surface area = $6(1-\varepsilon_e)/d_p$ (m^{-1})
d_p	pellet diameter (m)
K_s	solubility constant of $CaCO_3$ (mol^2/m^6)
f	activity factor (-), influenced by IS (Van Dijk and De Moel, 1983):

$$\log(f) = -\theta^2\{0.5\frac{\sqrt{IS}}{\sqrt{1000}+\sqrt{IS}} - 0.0002IS\}$$

IS	ionic strength $\cong 0.184\ EC$ (mol/m^3)
EC	electrical conductivity (mS/m)
θ	valency of ion (-)

With the crystallisation of calcium carbonate on the pellets, a new chemical equilibrium will be installed, the concentrations of carbonate, bicarbonate and carbon dioxide will be changed and consequently, the pH, the ionic strength and the activity factor will change. Both the concentrations of calcium and carbonate and the activity coefficient have influence on the driving force for crystallisation.

$$CO_2 + 2H_2O <=> H_3O^+ + HCO_3^- \qquad K_1 = (c_{H3O})(c_{HCO3})/(c_{CO2})$$

$$HCO_3^- + H_2O <=> H_3O^+ + CO_3^{2-} \qquad K_2 = (c_{H3O})(c_{CO3})/(c_{HCO3})$$

$$H_3O^+ + OH^- <=> 2H_2O \qquad K_w = (c_{H3O})(c_{OH})$$

$$Ca^{2+} + CO_3^{2-} <=> CaCO_3 \qquad K_s = (c_{Ca})(c_{CO3})$$

where

(c_{H30})	activity of hydrogen ion in water (mol/m^3)
(c_{HCO3})	activity of bicarbonate in water (mol/m^3)
(c_{CO2})	activity of carbon dioxide in water (mol/m^3)
(c_{OH})	activity of hydroxide in water (mol/m^3)
(c_{Ca})	activity of calcium in water (mol/m^3)
(c_{CO3})	activity of carbonate in water (mol/m^3)
$K_{,w,s}$	thermodynamic equilibrium constants (mol^2/m^6)
$K_{1,2s}$	thermodynamic equilibrium constants (mol/m^3)

$(c) \quad = f * c$

$$\log(K_1) = -356.3094 - 0.06091964*T + 21834.37/T + 126.8339*\log T - 1684915/T^2$$

$$\log(K_2) = -107.8871 - 0.03252849*T + 5151.79/T + 38.92561*\log T - 563713.9/T^2$$

$$\log(K_w) = 22.801 - 0.010365*T - 4787.3/T - 7.1321*\log T$$

$$\log(K_s) = -171.9065 - 0.077993*T + 2839.319/T + 71.595*\log T$$

Figure 6.3 Reactions of the different compounds within the calcium carbonic acid equilibrium (Plumer and Busenberg, 1982)

To be able to calculate the concentration of carbonate and the activity factor over the height of the bed, the conservative parameters m-alkalinity (*m*), p-alkalinity (*p*) and basic ionic strength (*BIS*) are introduced.

$$m = c_{HCO3} + 2c_{CO3} + c_{OH} - c_{H3O} \qquad (\text{mol/m}^3)$$

$$p = -c_{CO2} + c_{CO3} + c_{OH} - c_{H3O} \qquad (\text{mol/m}^3)$$

$$BIS = IS - 2c_{CO3} - 0.5c_{HCO3} - 0.5c_{H3O} - 0.5c_{OH} \qquad (\text{mol/m}^3)$$

The effect of dosing 1 mol/m^3 NaOH increases both *p* and *m* by 1 mmol/l and *BIS* by 0.5 mmol/l, whereas crystallisation of 1 mol/m^3 $CaCO_3$ decreases *p* by 1 mol/m^3 and *m* and *BIS* by 2 mol/m^3.

Figure 6.4 m-alkalinity, p-alkalinity and basic ionic strength (Van Dijk and Wilms, 1991)

During the crystallisation process of calcium carbonate in the reactor the following equations are valid:

$$\frac{\partial c_{Ca}}{dt} = -\frac{Q}{A_T \varepsilon_e}\frac{\partial c_{Ca}}{\partial x} - k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$
$$\frac{\partial m}{dt} = -\frac{Q}{A_T \varepsilon_e}\frac{\partial m}{\partial x} - 2k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$
$$\frac{\partial p}{dt} = -\frac{Q}{A_T \varepsilon_e}\frac{\partial p}{\partial x} - k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$
$$\frac{\partial BIS}{dt} = -\frac{Q}{A_T \varepsilon_e}\frac{\partial BIS}{\partial x} - 2k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$
$$\frac{\partial c_{CaCO3}}{dt} = -\frac{Q_s}{A_T}\frac{\partial c_{CaCO3}}{\partial x} + \varepsilon_e k_T a\{c_{Ca}\, c_{CO3} - \frac{K_s}{f^8}\}$$

From m-alkalinity, p-alkalinity, *K1*-, *K2*- and *Kw*-value the concentrations of carbon dioxide, bicarbonate, hydrogen and carbonate in water (c_{CO3}) are calculated, resulting in values for ionic strength, activity and pH.

6.2.3 Characteristics of the fluidised pellet bed

To determine the crystallisation rate in a unit element, the specific surface area (a) of the pellets and consequently the diameter of the pellets (d_p) and the porosity (ε_e) over the height of the reactor must be known.

During fluidisation the head loss in the bed can be calculated with an empirical formula derived for the transition between laminar and turbulent flow and adapted from the formula of Carman-Kozeny (Fair et al., 1968, Van Dijk and Wilms, 1991) . For spherical pellets, the head loss in the pellet bed is calculated by:

$$H = \frac{260}{\mathrm{Re}^{0.8}}\frac{L_{b0}}{d_p}\frac{(1-\varepsilon_0)}{\varepsilon_0{}^3}\frac{u^2}{2g}$$

Where

H Head loss (m)

L_{b0} height of unexpanded bed (m)

ε_0 porosity of unexpanded bed (-)

Re Reynolds number (-), $\mathrm{Re} = \frac{1}{1-\varepsilon_0}\frac{u d_p}{\nu}$

ν kinematic viscosity (m^2/s)

When fluidisation occurs, the head loss in the pellet bed is equal to the submersed weight of the pellet bed:

$$(1-\varepsilon_0)L_{b0}\frac{\rho_p-\rho_w}{\rho_w}=130\nu^{0.8}\frac{L_e}{d_p^{\;1.8}}\frac{(1-\varepsilon_e)^{1.8}}{\varepsilon_e^{\;3}}\frac{u^{1.2}}{g}$$

where

$$(1-\varepsilon_0)L=(1-\varepsilon_e)L_e$$

so

$$\frac{\varepsilon_e^{\;3}}{(1-\varepsilon_e)^{0.8}}=130\frac{\nu^{0.8}}{d_p^{\;1.8}}\frac{u^{1.2}}{g}\frac{\rho_w}{\rho_p-\rho_w}$$

Taking into account that the pellets are not spherical, the following equation for the calculation of the expanded bed porosity can be adopted:

$$\frac{\varepsilon_e^{\;3}}{(1-\varepsilon_e)^{0.8}}=130\frac{\nu^{0.8}}{(\phi d_p)^{1.8}}\frac{u^{1.2}}{g}\frac{\rho_w}{\rho_p-\rho_w}$$

The hydraulic diameter is regularly smaller than the calculated and the relation of the two is given by the shape factor (ϕ).

The partial differential equations can be solved numerically by considering unit elements of a reactor (see figure 6.2). Assuming a unit element (i) of the reactor that has a fixed amount of pellets (N_p). The mass balance is determined by the transport of pellets from one unit element to the following and by the crystallisation of calcium carbonate on the pellets. During the growth of the pellets the height of the element increases.

From the initial diameter of the grains, the accumulated calcium carbonate mass in the unit element ($M_s=c_{CaCO3}.\Delta x.A_T.M_{CaCO3}$), the density of the calcium carbonate and the initial porosity of the fluidised bed, the pellet diameter (d_p) is calculated. From there the density of the pellets and the porosity (ε_e) are determined. Finally, the new height of the unit element is calculated (Δx). The sum of the heights of the unit elements is the total height of the expanded bed.

$$N = \frac{A_T \Delta x_0 (1-\varepsilon_0)}{\frac{1}{6}\pi\, d_{p0}^3}$$

$$M_s = \rho_s \left(\frac{1}{6}\pi . d_p^3 - \frac{1}{6}\pi\, d_{p0}^3\right) N_{pi} \Rightarrow d_p = \sqrt[3]{\frac{d_{p0}^3}{1 - \frac{M_s}{\rho\, A_T \Delta x_0 (1-\varepsilon_0)}}}$$

$$\rho_p = \frac{\rho_g \frac{1}{6}\pi\, d_{p0}^3 + \rho_s \frac{1}{6}\pi . (d_p^3 - d_{p0}^3)}{\frac{1}{6}\pi . d_p^3}$$

$$\frac{\varepsilon_e^3}{(1-\varepsilon_e)^{0.8}} = 130 \frac{\nu^{0.8}}{g} \frac{\rho_w}{\rho_p - \rho_w} \frac{u^{1.2}}{\phi\, d_p^{1.8}}$$

$$\Delta x = \frac{N_p \frac{1}{6}\pi\, d_p^3}{A_T . (1-\varepsilon_e)} = \frac{d_p^3}{d_{p0}^3} \frac{(1-\varepsilon_0)}{(1-\varepsilon_e)}$$

Where

M_s	mass of crystallised calcium carbonate in unit element (kg)
M_{CaCO3}	molecular weight calcium carbonate (kg/mol)
N_p	number of grains in unit element (-)
Δx_0	height of unit element in a non-expanded clean bed (m)
Δx	height of unit element i in an expanded bed (m)
ε_0	porosity of non-expanded clean bed (-)
ε_e	porosity of expanded bed (-)
d_{p0}	initial diameter of grains (m)
ρ_p	density of pellet in unit element (kg/m^3)
ρ_s	density of calcium carbonate (kg/m^3)
ρ_g	density of grain (kg/m^3)
ρ_w	density of water (kg/m^3)

6.3 Materials and methods

6.3.1 Modelling approach

The model is developed within the Stimela environment (see chapter 3).

The model consists of:

- Input disturbance variables:
    - water flow Q (m^3/s)
    - water temperature T (K)
    - calcium concentration c_{Ca} (mol/m^3)
    - m-Alkalinity m (mol/m^3)
    - p-Alkalinity p (mol/m^3)
    - electrical conductivity EC (mS/m)
- Input manipulated variables:
    - dosage of caustic soda (NaOH) (mol/m^3)
    - height of seeding material in reactor (m)
    - calcium carbonate velocity u_s (m/s)
- State variables:
    - calcium concentration c_{Ca} (mol/m^3)
    - calcium carbonate concentration c_{CaCO3} (mol/m^3)
    - m-Alkalinity m (mol/m^3)
    - p-Alkalinity p (mol/m^3)
    - basic ionic strength BIS (mol/m^3)
- Output water quality variables:
    - water flow Q (m^3/s)
    - water temperature T (K)
    - calcium concentration c_{Ca} (mol/m^3)
    - m-Alkalinity m (mol/m^3)
    - p-Alkalinity p (mol/m^3)
    - electrical conductivity EC (mS/m)
- Extra output variables:
    - pressure drop over the reactor
    - height of the expanded bed
    - pellet diameter over the height of the reactor
- Additional variables:
    - pellet diameter d_p (m)
    - pellet bed porosity ε_e (-)

  - height of unit element Δx (m)
- Physical parameters:
  - surface area of reactor A_T (m^2)
  - height of pellet reactor L_R (m)
  - diameter of seeding material d_{p0} (m)
  - density of seeding material ρ_{p0} (kg/m^3)
  - initial bed porosity ε_0 (-)
  - hydraulic shape factor of pellets ϕ (-)
  - density of calcium carbonate ρ_s (kg/m^3)
- Calibration parameters
  - kinetic constant k_T (m^4/mol.s)
  - number of unit elements (-)

The initial condition of the model is determined by the amount of calcium carbonate that is accumulated in the reactor. At start-up of the reactor the calcium carbonate concentration c_{CaCO3}=0 mol/m^3 and the calcium concentration, m-alkalinity, p-alkalinity and basic ionic strength is equal to the input water quality after dosing of caustic soda.

6.3.2 Description of WTP Weesperkarspel Amsterdam Water Supply

The model for the pellet softening process was tested on data from one of the softening reactors of WTP Weesperkarspel of Amsterdam Water Supply.
The reactor has the following characteristics:

- Surface area of reactor A_T	5.3 m^2
- Maximum bed height	5 m
- Grain size of seeding material d_{p0}	0.28 10^{-3} m
- Density of the seeding material ρ_{p0}	4114 kg/m^3

In addition the following assumptions were made

- Initial fixed bed porosity ε_0	0.41
- Hydraulic shape factor of pellets ϕ	0.7
- Density of calcium carbonate ρ_s	2730 kg/m^3
- Kinetic constant k_T	$(0.0255\ 10^{-3})(1.053)^{T-293}$ m^4/mol.s
- Number of unit elements	7

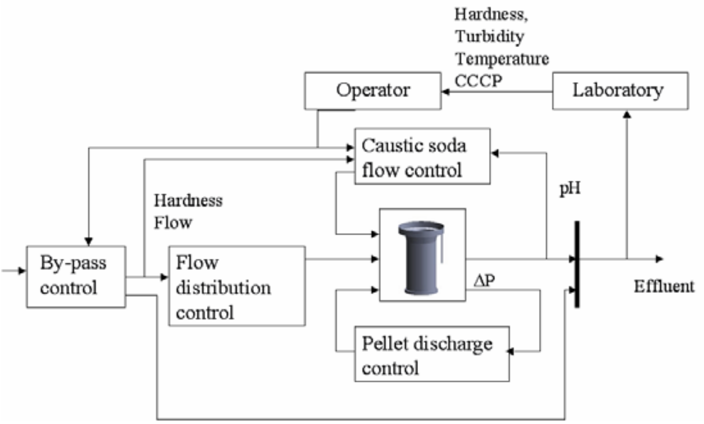

Figure 6.5 Representation of present control at WTP Weesperkarspel

At WTP Weesperkarspel, depending on temperature, the by-pass ratio and dosing of caustic soda (NaOH) in the pellet reactor are adjusted in such a way that the hardness of the mixed effluent is 1.5 mol/m^3. Pellet removal is controlled by the hydraulic resistance of the filter bed (pressure drop). The hydraulic resistance is kept between 1.65 and 1.72 m. The pH, flow, temperature, hardness and hydraulic resistance are measured every minute, while calcium, bicarbonate, super-saturation, pellet diameter, bed height are measured at longer intervals (daily to weekly).

There are four main controllers that regulate the softening process (see figure 6.5, Wuister, 2003):

1. The flow and its distribution over the reactors
2. The by-pass controller that is set manually.
3. The caustic soda controller dose based on the desired effluent calcium concentration, the water flow, the effluent pH, the by-pass ratio, the temperature and a manual correction. The set point is calculated using an empirical formula.
4. The pellet discharge controller, which keeps the total pressure drop over the reactor between 1.65 and 1.72 m.

In summer, this practice results in higher by-pass regimes and higher NaOH dosage per reactor. In winter, less by-pass is applied and the NaOH dose per reactor are lower. To keep the super-saturation at acceptable levels, the maximum pellet size is decreased in winter in order to increase the specific surface area of the fluidised bed. In summer the contrary occurs.

6.4 Verification of model

The performance of the model is verified with routinely collected data of the year 2002 from one of the softening reactors of WTP Weesperkarspel. The overall performance of the reactor over the year 2002 is demonstrated in figure 6.6. During simulation the pellet discharge is kept as a constant. Measurements of bed height, hydraulic shape factor and the amount of seeding material in the reactor were not available and are estimated.

The results of the model indicate that they are in the range of the accuracy of the measuring devices. It can be concluded that the response to flow, caustic soda flow and water quality changes is fairly good. In the first 50 days the pH, alkalinity and calcium concentration is overestimated. This is due to start-up. The model starts with a clean bed, whereas in real life the reactor has a history. Between day 260 and 270 a flow interruption occurred. For the calculations the ionic strength must be known, but it is not measured directly. Therefore, the indirect measurement of electrical conductivity is used to estimate the ionic strength. The relation between ionic strength and electrical conductivity was found to be in the range of 0.15 and 0.16.

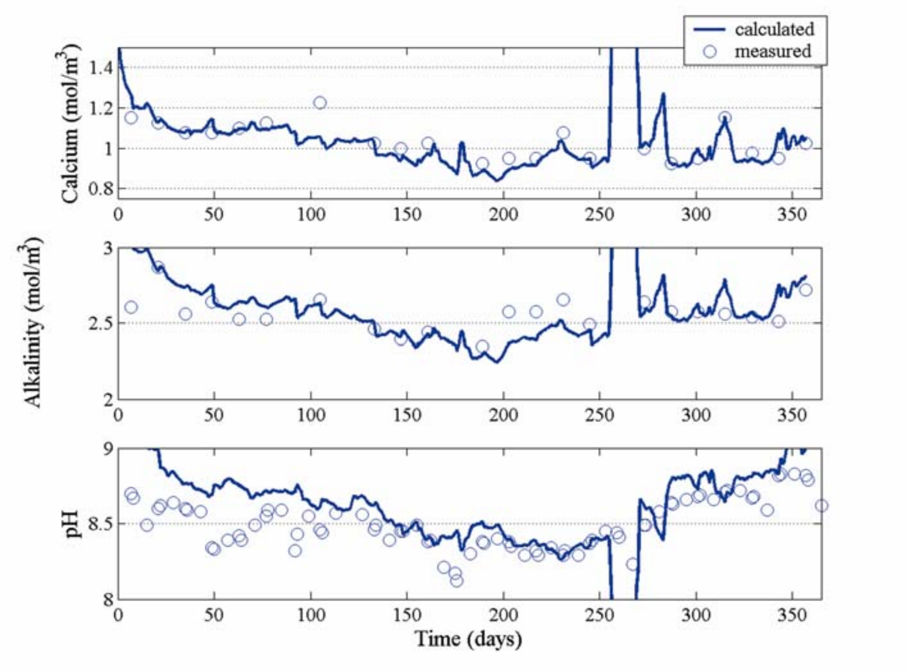

Figure 6.6 Validation of model on data from WTP Weesperkarspel (2002)

It must be stressed that deviations in the calculation are not always a matter of modelling. They could have been caused by on-line sensors being out of the calibration range or operational changes. In addition, data registration problems could also have been occurred.

During the calibration exercise it was found that the caustic soda flow was not correctly measured and therefore a correction factor was introduced (see figure 6.7).

The caustic soda dose is calculated by the following equation:

$$NaOH = \frac{Q_{NaOH}}{Q + Q_{NaOH}} . \frac{\rho_{NaOH} . \sigma t_{NaOH}}{M_{NaOH}}$$

Where

$NaOH$	caustic soda dose in (mol/m^3)
Q_{NaOH}	caustic soda flow in m^3/s
Q	water flow in m^3/s
ρ_{NaOH}	density of caustic soda solution in kg/m^3 (=1250)
σt_{NaOH}	strength of the caustic soda solution in kg/kg (=0.25)
M_{NaOH}	molecular weight of caustic soda g/mol (= 40)

From theory it can be concluded that

$$m_{out} = m_{in} + NaOH - 2(c_{Ca,out} - c_{Ca,in})$$

Where

m	m-alkalinity (mol/m^3)
c_{Ca}	calcium concentration in water mol/m^3

From the measurements it can be concluded that m_{out}=2.57 mol/m^3, m_{in}=3.33 mol/m^3 and ($c_{Ca,in}$-$c_{Ca,\mathrm{out}}$)=0.975 mol/m^3, resulting in a calculated caustic soda dose $NaOH$ of 1.18 mol/m^3, which is much less than the measured dose of 1.3 mol/m^3 $NaOH$. This indicates that the caustic soda dosing measurement is hampering.

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Figure 6.7 Explanation of hampering measurements of caustic soda flow

6.5 Optimal operation of pellet softening

Optimal operation is achieved when minimal super-saturation in the mixed effluent is obtained using the infrastructure installed, avoiding pH correction at the effluent and minimising the caustic soda dose.

Super-saturation is expressed as *TCCP* (theoretical calcium carbonate crystallisation potential). This is the concentration of calcium (mol/m^3) that should be crystallised to obtain water in chemical equilibrium.
To obtain the lowest *TCCP* in the effluent of the reactor, the fluidised bed height must always be kept at its maximum. The bed height depends on the amount of pellets in the reactor, water flow through the reactor, pellet diameter (and density) and water temperature. The water flow through the reactor depends on the water demand, the number of reactors in operation and the by-pass ratio. The lower the flow through the reactor (and thus the higher the by-pass ratio), the more pellets can be maintained in the reactor, but the deeper the softening in the reactor must be.

The *TCCP* in the effluent of the reactor is further influenced by the dose of NaOH and by the available precipitation surface area (number of grains, diameter of the grains). The mixture of two waters in carbonic acid equilibrium will be aggressive to calcium carbonate. The slightly super-saturated effluent of a pellet reactor (positive *TCCP*) that is mixed with by-pass water in equilibrium can thus result in a mixture in chemical equilibrium.
The allowable degree of super-saturation in the effluent of the reactor depends thus on the by-pass water quality and by-pass ratio.

Optimal operation of the pellet softening reactors is determined by by-pass ratio, pellet discharge velocity, number of pellets in the reactor, dosing of caustic soda and number of reactors in operation. All these variables represent a monetary value:

- By-pass ratio, bed height and pellet discharge velocity influence the super-saturation in the mixed effluent that in its turn influences dosing of caustic soda, dosing of acids for neutralisation or the regeneration frequency of the subsequent carbon filter
- Pellet velocity influences the discharged grain size and thus the amount of seeding material per kilo pellets
- Number of reactors in operation represents maintenance costs.
- Number of reactors in operation and the by-pass ratio influence the energy costs.

For a stationary situation the optimisation objectives can thus be formulated in the following cost function *J*:

$$J = \sum w_1 (c_{Ca_{ref}} - c_{Ca})^2 + w_2 (TCCP_{ref} - TCCP)^2 + w_3 (N_R) \quad + w_4 (d_{p,ref} - d_p)^2$$

Where c_{Ca} is the calcium concentration in the effluent, *TCCP* is the super-saturation, N_R is the number of reactors in operation, d_p is the released pellet size and w_i are weighing factors specifying the relative importance of the different criteria.

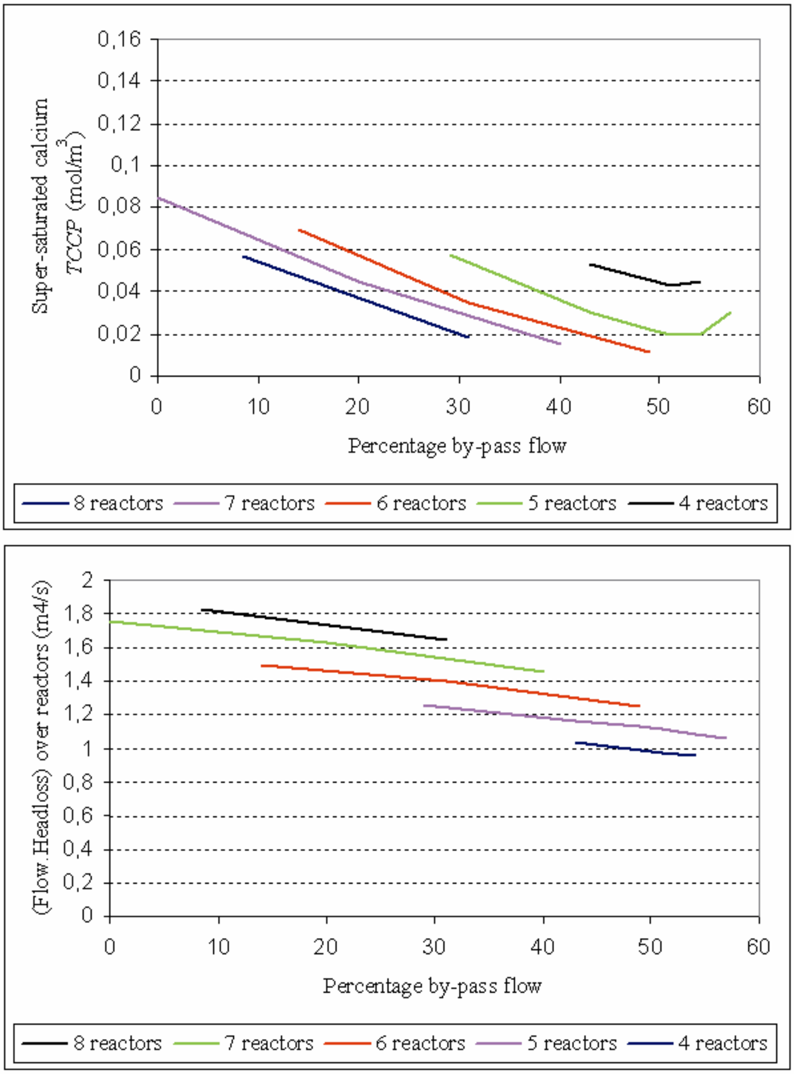

Figure 6.8 Operational scenarios for softening at WTP Weepserkaspel, flow 3500 m^3/h, 10 °C, (c_{HCO3} = 204 g/m^3, c_{Ca}=80 g/m^3, pH=7.61, *EC*=53 mS/m)

As an example different operational scenarios at WTP Weesperkarspel are simulated for a total (average) flow of 3500 m^3/h at a temperature of 10 °C (see figure 6.8). In all scenarios the total hardness of the mixed effluent is kept at 1.5 mol/m^3 and the fluidised bed height at the maximum of 5 m. In addition, three flow velocities of 94, 75 and 57 m/h are used during the calculations and the maximum pellet diameter is kept at 1.10^{-3} m. From the scenario analysis of this example it can be concluded that the super-saturation of the mixed effluent is minimal at a by-pass ratio of about 50% with a maximum of reactors in operation (in this case 6). With this by-pass ratio more reactors cannot be operated, because of operational constraints with respect to flow velocity through the reactor. The energy consumption of six reactors in operation is about 10% higher than with 5 reactors in operation, but the super-saturation in this case is twice the super-saturation with 6 reactors in operation. For a lower temperature the same trend is observed (see figure 6.9).

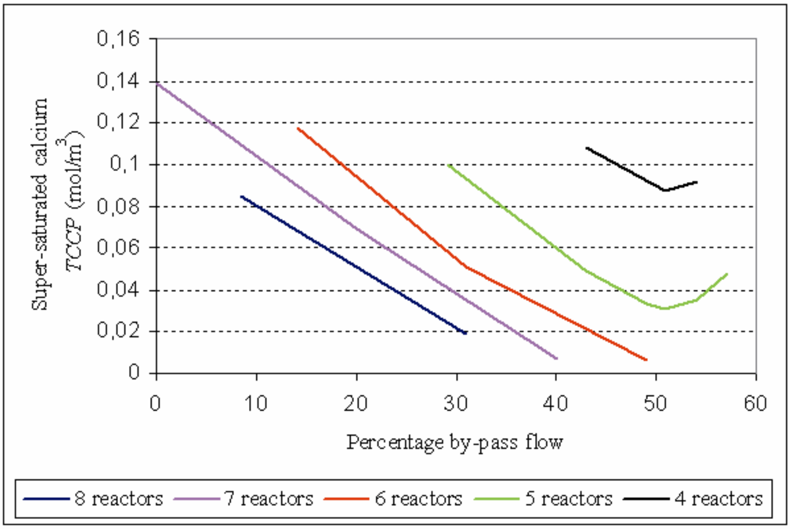

Figure 6.9 Operational scenarios for softening at WTP Weesperkarspel, flow 3500 m^3/h, 1.2 °C, (c_{HCO3} = 208 g/m^3, c_{Ca} =80 g/m^3, pH=7.59, *EC*=52.4 mS/m)

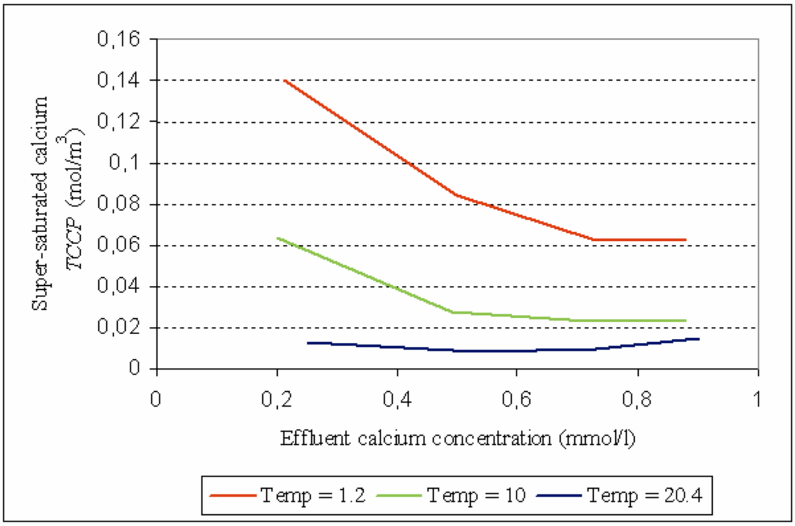

Figure 6.10 Effluent calcium concentration of single reactor related to *TCCP*, flow 300 m^3/h

The optimal softening depth is not always the optimal point of an individual reactor. The optimum for the case of WTP Weesperkarspel is a reactor effluent calcium concentration of about 0.5 mol/m^3 (resulting from a by-pass ratio of 50%: influent is 2 mol/m^3 and mixed effluent should be 1.25 mol/m^3). From figure 6.10 follows that mainly in colder waters a higher effluent concentration of an individual reactor gives lower super-saturation. However, because in these cases the by-pass flow is lower, this is not the optimal point for the mixed effluent.

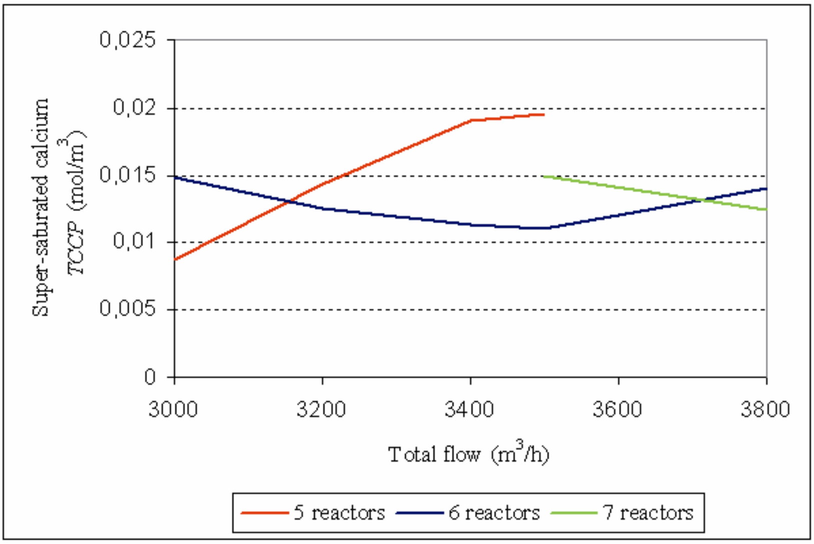

Figure 6.11 Total flow related to number of reactor in operation and super-saturation at 10°C.

When water flows need to be treated that are higher or lower than the average 3500 m^3/h, the operational action must be determined. Either the water flow through the reactor or the by-pass flow can be changed. Using the super-saturation as the leading criterion, it can be concluded from figure 6.11 that, at 10 °C, operating 6 reactors with a by-pass ratio between 43 and 50% and a flow through the reactor between 300 and 310 m^3/h is optimal with flows between 3200 m^3/h and 3700 m^3/h.

6.6 Discussion

It can be concluded that modelling pellet softening will lead to a different, optimal operation and change present practice. Nowadays the control is mainly based on head loss that is kept between 1.67 and 1.72 m (see figure 6.10). For cold water and high flows through the reactor this pressure drop is well chosen (as upper boundary). However, for different circumstances higher pressure drops can be allowed, resulting in more seeding material in the reactor and thus a better performance. For flows through a reactor of 300 m^3/h, the pressure drop can be maintained between 2.3 and 2.9 m (depending on temperature), using maximally the installed capacity (see figure 6.12).

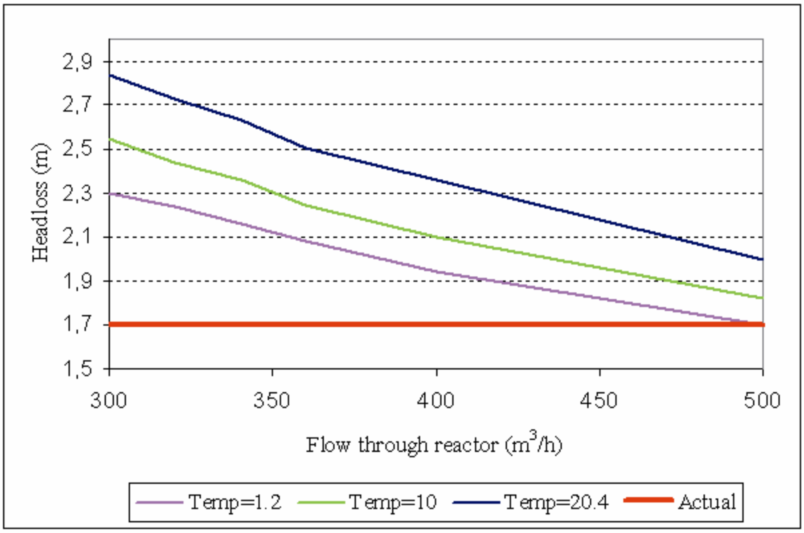

Figure 6.12 Head loss as a function of flow through the pellet reactor

Due to the high costs and environmental impact of the use of chemicals, in practice, the *TCCP* in the mixed effluent must be minimal. This implies that the maximal by-pass ratio and the minimal flow through the reactor (under the prevailing boundary conditions) must be chosen. The reactors must be filled completely with fluidised pellets. To determine the maximal by-pass ratio and the fluidised bed height the model is used. With this approach, it is concluded that during average flow not all of the installed reactors should be used (6 out of 8).

Compared to present operation up to 5% of the caustic soda could be saved and a reduction in *TCCP* of up to 0.05 mol/m^3 could be obtained, diminishing the acid dosing for pH correction. This means a reduction of about € 40.000,- per year or 0.15 ct/m^3 water produced.

More important, however, is the increase in capacity of the system, using the proposed approach by allowing higher by-pass flows. It is concluded that during average flow, with the lowest super-saturation, the overcapacity is about 33% (6 of the 8 reactors in operation). A higher flow could either be treated by the 6 reactors accepting a higher effluent super-saturation or by one of the spare reactors, still allowing a reduction of one reactor.

6.7 Future work

In drinking water treatment the water quality and the water flow change constantly and for every circumstance new optimal states must be found. A new state cannot be reached instantaneously, because of the dynamic behaviour of the process. In case of a decrease in flow in the reactor, new grains must be added to the reactor and these grains must grow into pellets. In case of an increase in flow a number of pellets must first be removed before the flow increase, to avoid wash out from the top of the reactor. The removal rate of pellets per reactor and the head loss corresponding to the flow through a reactor full of fluidised pellets can be calculated with the model. Therefore, in the context of the project PROMICIT at Amsterdam Water Supply, a model predictive controller will be designed and tested at an automated pilot plant. On-line data will be collected and sent to a PC. After determining the set points, they are given through to the controlled devices.

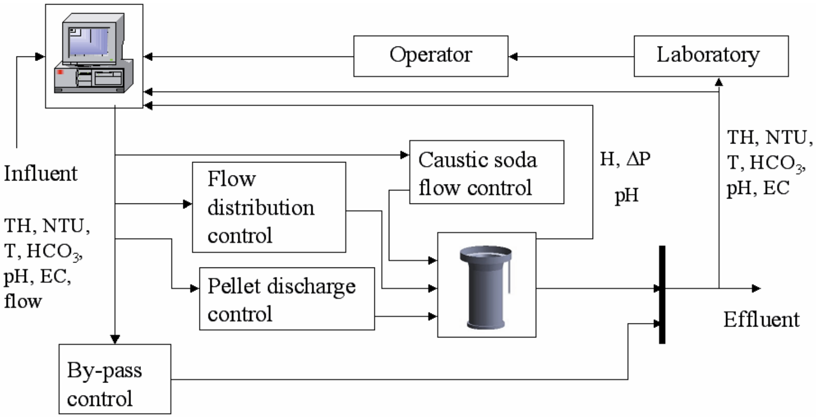

Figure 6.13 Proposed control for pellet softening at WTP Weesperkarspel

The quality of the by-pass flow is also subject to decision-making. An adapted treatment of the by-pass flow can for example lead to lower super-saturation, asking for an integral approach to the control of a drinking water treatment plant. The interaction of the different treatment processes and the impact on softening is also part of the PROMICIT project and will further be elaborated.

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7 CONCLUSIONS

7.1 Improving operation of drinking water treatment

7.1.1 Case studies

In the present thesis the improvement of operation of drinking water treatment is illustrated with three case studies of the "post-conventional" processes ozonation, granular activated carbon (GAC) filtration and pellet softening.

From the first case study, it is concluded that in actual ozonation practice the CT-value is underestimated, because the bubble column is not accounted for. The contribution of the bubble columns in the pilot plant Weesperkarspel of Amsterdam Water Supply, was, at 20°C, 30% of the total CT-value for the counter current flow and 80% for the co-current flow configuration. In practice, a higher overall CT-value is present than supposed and thus a greater disinfection capacity is available than expected. Thus, if the guarantee of disinfection is linked to CT-value, dosing of ozone can be reduced when, in addition to the contact chambers, concentrations and residence time in the bubble column are taken into account.

In the second case study, different scenarios are evaluated, comparing pseudo moving bed with operation in parallel and assuming a better planning of regeneration of the filters. At WTP Reijerwaard it is concluded that parallel operation will lead to shorter filter run times (2 years instead of 2.5 years), but has as advantage that operation becomes less complicated and that the system can treat a greater water flow. For water treatment plant (WTP) Rodenhuis of Hydron ZH, it is concluded that prevailing regeneration practice of granular activated carbon filtration (GAC), in economic terms, is sub-optimal. The average value of the target water quality parameter, in this case bentazon, is far below the allowable values. The number of regenerations of the activated carbon (GAC) could be reduced by 20% (1 regeneration less per year). The activated carbon filters can be less frequently regenerated when the target parameter, determining the effluent water quality, is kept constantly along the guideline level. Regenerations are the main operational costs of the process and, therefore, considerable economic and environmental benefits can be obtained when the filter run times are prolonged.

Based on the model evaluations of the pellet softening reactors at WTP Weesperkarspel of Amsterdam Water Supply, in the third case study, a change in operation was proposed in order to obtain a better water quality (less super-saturation). Therefore, the by-pass ratio and the fluidised bed height should be maximised and the flow through the individual reactors minimised. The head loss over the reactor is in that case not constant and depends on water velocity through the reactor and on water temperature. With this approach, it is concluded that during average flow not all of the installed reactors should be used (6 out of 8). In the softening process, an improvement in effluent water quality also means a saving of chemicals, leading to a reduction in operational costs and environmental emissions. With an improved operation the caustic soda dosage could be reduced with about 5-10% and almost the total amount of hydrochloric acid for pH correction could be saved.

7.1.2 Role of models in operation

With advances in computer science, PC-technology and modelling techniques, there are new possibilities to use the abundant availability of data to improve operation of drinking water treatment, leading to better drinking water quality and/or reduction in operational costs and/or reduction in environmental emissions. Moreover, the insight in the process will be increased, resulting in more confidence in the performance of the treatment plant. Interventions can be planned and changes can be anticipated.

Modelling for operation gives more information about the state of the process. In real life not all parameters can be monitored on-line or with frequent intervals. Examples are: ozone concentration at different places in the bubble columns and contact chambers, degree of loading of the activated carbon, pellet size in the softening reactor. In order to be able to judge the state of the process constantly model predictions are indispensable. Well-calibrated models can even lead to virtual monitoring of the effluent water quality, resulting in a reduction of analysis costs.

Using models to evaluate the operational interactions can also lead to more knowledge about the process, without performing costly pilot plant research. Events that are nowadays not understood can be analysed using primarily data from the full-scale plant. Operators become, thus, more involved in ongoing research, which can even lead to alternative set-up of the treatment scheme or more focused pilot plant research. For example, from the analysed data of WTP Weesperkarspel of Amsterdam Water Supply the influence of the seasonal effects of the water quality on the softening process was obvious. Not only does the water temperature influence the reaction velocity and the bed expansion of the fluidised bed, the incoming super-saturation of the water also changed. This gave rise to a discussion on the integral approach of pH control throughout the drinking water treatment plant.

During the modelling experiments fundamental questions can be raised about the functioning of the process, leading to new research questions. A fruitful exchange of science and practice will then be developed. For example, for the determination of the maximal filling of the softening reactor, a relation between the water flow, pellet size distribution and head loss must be found. Standard models did not suit. Therefore, a separate study was executed to find a description for the bed expansion of pellets in a softening reactor.

Finally, the use of models in operation of drinking water treatment will lead to a stable process, avoiding rapid changes in produced water flow, distribution of flow over the different units and dosing of chemicals. The stable operation will be advantageous for the process leading to fewer troubles in the process. For example, in the softening reactors so-called “cauliflowers” (high calcium carbonate concentrations) and “mucus” (fines) occur. This is probably due to local overdosing. When operation can be smoothened and the best dose can be calculated, it is expected that these troubles will be tackled.

7.2 Use of numerical simulation tool in drinking water treatment

Conventional, static modelling for design optimisation was mainly focussed on the determination of the dimensions of the process, in relation to the influent quality and the required effluent quality. The present approach focuses on simulation, assuming the dimensions of the process and the process parameters, calculating the consequences for the product.

For the second approach more a-priori knowledge of the process is needed and the approach facilitates training and education. Simulation can also be used for design optimisation. Although the calculation times will be longer than with the conventional, static approach, the advantage is that operation and variations in time can be evaluated in the design. This will result in an overall optimisation rather than an optimisation on the worst-case scenario.

Simulation is a useful tool to improve operation. In the present study a numerical simulation tool is used for (dynamic) modelling of the processes. For slow reacting processes such as filtration, granular activated carbon filtration and pellet growth in the softening reactor dynamic modelling is a prerequisite. The consequence of changing influent concentrations and water flow through the system can be evaluated in relation to the state of the system. In this way operators can constantly evaluate alternative operational scenarios and choose the best option. Rapid reacting processes such as aeration, ozonation and pH adjustment do not strictly need a dynamic approach. Because the time span is short in relation to the residence time in intermediate storage reservoirs, the effect of the delayed effluent changes can be neglected. However, numerical simulation of these processes may substitute iterations that are used to calculate the equilibrium.

Using the same environment for process control, training and design has the advantage that communication between operators, designers and researchers is promoted. The use of web based applications like www.stimela.com is even further stimulating this interaction.

7.3 Future work

7.3.1 Improved operation in practice

At WTP Weesperkarspel of Amsterdam Water Supply, the ozone dosing is adjusted twice a year, reducing the dosing during the summer period, because of abundant bacterial growth in the GAC filters. However, the decay of ozone is higher when water temperature increases, resulting in even lower CT-values than in winter. Operation should focus on maintaining CT-value at a required level and thus guaranteeing disinfection, taking into account changing water quality parameters as temperature and UV-absorbance. The use of an ozonation model will help operators to determine CT-value in every instant and to evaluate the necessary ozone dosing, leading to a better proved water quality and, occasionally, a lower ozone dose. The model based decision supported operation of the ozonation process at WTP Weesperkarspel is scheduled for 2005.

Based on the model studies for pellet softening, research is being executed at the pilot plant Weesperkarspel of Amsterdam Water Supply to further validate the model and to test the proposed operational scenarios. Therefore, the pilot plant is being automated and equipment is built in for on-line measurement of bed height, head loss and influent and effluent water quality. The model will then be used for the development of a model predictive controller for on-line optimal control of the pellet softening process.

7.3.2 Interaction of drinking water treatment processes

In many industrial applications the main process is concentrated in one reactor. In drinking water, however, many different parameters are addressed and different treatment processes must be put in series. For some parameters this means that a multi-barrier exists: pathogenic micro-organisms for example are removed by floc formation and removal, filtration, disinfection (ozone, chlorine and UV) and slow sand filtration in the same treatment train. One process is normally optimised for one specific objective. Floc formation, for example, is normally designed to remove turbidity. The removal of natural organic matter or pathogenic micro-organisms is seen as a co-lateral effect. The interaction of the processes and overall efficiency is normally not taken into account. The sum of the optimised individual processes is considered to be the optimised system. In practice, this can lead to sub-optimal performance.

In the present work emphasis is given to modelling of individual processes and the interaction of the treatment processes is not taken into consideration. The designs of treatment processes are also based on the individual performance with pre-set boundary conditions. Treatment processes, however, are influenced by the performance of preceding processes. For example, ozonation is the main barrier for pathogenic micro-organisms. Part of the ozone is consumed by natural organic matter (NOM) and will not be available for disinfection. A lower removal of NOM in the pre-treatment, will lead to higher ozone doses to maintain the required disinfection level.

Taking into account the developments in sensoring, automation and computation, it is a challenge to improve quality and reliability of the treatment plants and to make maximal use of the installed infrastructure, postponing new investments. It is, therefore, assumed that an integral approach of the entire treatment plant can lead to more efficient operation. Recently (January 2003), Amsterdam Water Supply, Delft University of Technology, DHV Water B.V. and ABB B.V. started the 'PROMICIT' project, which is subsidised by Senter, Ministry of Economic Affairs, the Netherlands. The aim is to achieve a breakthrough in drinking water quality control by developing an integral, dynamic model of the total water treatment plant and the use of this model as a basis for integral, on-line, quality control. WTP Weesperkarspel of Amsterdam Water Supply is subject of this project.

SUMMARY

Operation of drinking water treatment plants is nowadays based on experience. Water quality is monitored to prove that guidelines are met and, sometimes, laboratory tests are performed to determine e.g. the dosage of chemicals. All these data, however, are scarcely used to improve day-to-day operation and disappear in the cellars of the water company. By using modelling in combination with on-line monitoring and real-time control, the operation can be improved, resulting in better and more stable water quality, better use of the installed infrastructure, lower treatment costs and/or reduction of environmental emissions.

The objective of the research is to demonstrate that the operation of dinking water treatment facilities can be improved through modelling. Continuous model evaluation of different operational scenarios will lead to improved operation that varies in time. Therefore, phenomenological models are used that are based on numerical integration of partial differential equations, describing the process and the dynamic behaviour of the processes. The models are elaborated within the modelling environment Stimela, which is programmed in Matlab/Simulink™.

The different processes in drinking water treatment have similar mechanisms and can be described with similar partial differential equations, based on the advection-dispersion model. Basic equations are given for transport of compounds through a reactor, transfer to a gas or solid phase, decay of the compound and mass balance between the water and the gas or solid phase

To illustrate the value of modelling for operational improvement, three cases are elaborated. The cases describe the “post-conventional” processes ozonation, granular activated carbon filtration (GAC) and pellet softening that are used in the Netherlands for polishing the drinking water after conventional treatment.

Decimal elimination of pathogenic micro-organisms during ozonation is linked to the CT-value (based on ozone concentration and residence time). The CT-value is normally only determined for contact chambers and the effect of the bubble column is neglected. In the first case study, ozone profiles are obtained with data from counter current flow and co-current flow reactors of the pilot plant Weesperkarspel at Amsterdam Water Supply and with these data a model for bubble columns is calibrated. The model is based on differential equations that describe the flow of water and gas through the reactor, the transfer of ozone from the gas phase to the water, the slow and rapid decay of ozone in water. The contribution of the bubble columns in the pilot plant was, at 20^{o}C, 30% of the total CT-value for the counter current flow

and 80% for the co-current flow configuration. In practice a higher overall CT-value is present than supposed and thus a greater disinfection capacity is available than expected. If the guarantee of disinfection is linked to CT-value, dosing of ozone can be reduced when, in addition to the contact chambers, concentrations and residence time in the bubble column are taken into account.

In the second case study the removal of bentazon by activated carbon filters of two locations, drinking water treatment plants (WTP) Rodenhuis and Reijerwaard of Hydron ZH, is modelled. The activated carbon filters are installed in series of two filters in a pseudo moving bed configuration. From pilot and full-scale plant data, the run time of granular activated carbon filters is calculated under changing influent water quality and is compared to existing operation practice. The model of the GAC is based on differential equations that describe the transport of micro-pollutants through the filter bed, the transfer of micro-pollutants from the water to the solid phase and accumulation of micro-pollutants in the pores of activated carbon grains. The model is fitted with data of the pilot plant and the WTP at Rodenhuis and validated with data from WTP Reijerwaard, where the preloading with natural organic matter is higher. Different scenarios are evaluated assuming a better planning of regeneration of the filters and comparing pseudo moving bed with operation in parallel. At WTP Reijerwaard it is concluded that parallel operation will lead to shorter filter run times (2 years instead of 2.5 years), but has as advantage that operation becomes less complicated and that the system can treat a greater water flow. For WTP Rodenhuis it is concluded that prevailing regeneration practice of granular activated carbon filtration (GAC), in economic terms, is sub-optimal. The average value of the target water quality parameter, in this case bentazon, is far below the allowable value. The number of regenerations of the activated carbon (GAC) could be reduced by 20% (1 regeneration less per year). Regenerations are the main operational costs of the process and, therefore, considerable economic as well as environmental benefits can be obtained when the filter run times are prolonged.

In the third case study the pellet softening process is modelled and evaluated for WTP Weesperkarspel of Amsterdam Water Supply, where for softening caustic soda is dosed. The objective of the study was to find an optimisation in operation, minimising super-saturation of calcium ions in the mixed effluent of the reactors. Data were collected from one pellet softening unit of the WTP. A model was developed based on partial differential equations describing the flow through the reactor, crystallisation of calcium carbonate on the pellets, growth of the pellets, transport of the pellets through the reactor, filter bed expansion as a function of flow and pellet size and hydraulic head loss over the reactor. Based on the model evaluations a change in operation was proposed in order to obtain a better water quality (less super-saturation). Therefore, the by-pass ratio and the fluidised bed height should be maximised and the flow through the individual reactors minimised. The head loss over the reactor is in that case not constant and depends on water velocity through the reactor and on water temperature. With this approach, it is concluded that during average flow not all of the installed reactors should be used. In the softening process, an improvement in product water quality also means a saving of chemicals, leading to a reduction in operational costs and environmental emissions. With an improved operation the caustic soda dosage could be reduced with about 5-10% and almost the total amount of hydrochloric acid for pH control could be saved.

Generally it was concluded that with advances in computer science, PC-technology and modelling techniques, there are new possibilities to use the abundant availability of data to improve operation of drinking water treatment, leading to better drinking water quality and/or reduction in operational costs and/or reduction in environmental emissions. Moreover, the insight in the process will be increased, resulting in more confidence in the performance of the treatment plant. Interventions can be planned and disturbances can be anticipated. Modelling for operation gives more information about the state of the process. In real life not all parameters can be monitored on-line or with frequent intervals. Well-calibrated models can even lead to virtual monitoring of the product water quality, resulting in a reduction of analysis costs. Using models to evaluate the operational interactions can also lead to more knowledge about the process, without performing costly pilot plant research. Events that are nowadays not understood can be analysed using primarily data from the full-scale plant. Operators become, in this way, more involved in ongoing research, resulting in more focused pilot plant research and which can even lead to alternative set-up of the treatment scheme. The use of models in operation of drinking water treatment will lead to a stable process, avoiding rapid changes in produced water flow, distribution of flow over the different units and dosing of chemicals. The stable operation will lead to fewer troubles in the process.

In future, work will be executed related to the implementation of the models in practice. They will be used for model based decision support in operation and integrated in model predictive controllers for on-line, optimised, automated control. In addition, the individual models will be linked to each other, resulting in an integral approach of the entire treatment plant for even more efficient operation.

SAMENVATTING

De bedrijfsvoering van drinkwaterzuiveringsinstallaties is gebaseerd op ervaring. De waterkwaliteit wordt gemonsterd om te bewijzen dat de kwaliteitsnormen en -richtlijnen worden gehaald en soms worden laboratoriumtesten uitgevoerd om bijvoorbeeld de dosering van chemicaliën te bepalen. Al deze gegevens worden echter zelden gebruikt om de dagelijkse besturing te verbeteren en verdwijnen in de kelders van het waterleidingbedrijf. Door het gebruik van modellen, in combinatie met on-line monitoren en real-time besturing, kan de bedrijfsvoering worden verbeterd. Dit zal leiden tot een betere en stabielere waterkwaliteit, beter gebruik van de geïnstalleerde infrastructuur, lagere zuiveringskosten and een verlaging van de uitstoot in het milieu.

Het doel van het promotieonderzoek is om aan te tonen dat de bedrijfsvoering van drinkwaterzuiveringsinstallaties verbeterd kan worden door gebruik te maken van modellering. Simulaties van verschillende bedrijfsvoeringscenario's zullen leiden tot een verbeterde bedrijfsvoering die varieert in de tijd. Daarom worden fenomenologische modellen gebruikt die zijn gebaseerd op het numeriek integreren van partiële differentiaalvergelijkingen, die het proces en het dynamische gedrag van het proces beschrijven. De modellen zijn uitgewerkt in de modelleeromgeving Stimela, die geprogrammeerd is in Matlab/Simulink™.

De verschillende stappen in de drinkwaterzuivering hebben vergelijkbare mechanismen en kunnen worden beschreven met vergelijkbare partiële differentiaalvergelijkingen, die gebaseerd zijn op het advectie-dispersie model. Vergelijkingen zijn gegeven voor het transport van stoffen door een reactor, overdracht naar een gas- of een vaste fase, afbraak van de stof en de massabalans tussen het water en de gas- of vaste fase.

Om de waarde van het modelleren te illustreren, zijn drie praktijkvoorbeelden uitgewerkt. De voorbeelden beschrijven de "post-conventionele" processen ozonisatie, aktieve koolfiltratie (GAC) en ontharding met een korrelreactor. Deze processen worden in Nederland gebruikt om het drinkwater, na de conventionele zuivering, verder te verbeteren.

Decimale eliminatie van pathogene micro-organismen tijdens de ozonisatie is gekoppeld aan de CT-waarde (gebaseerd op ozonconcentratie en verblijftijd). De CT-waarde wordt normaliter alleen berekend voor de contactkelders en het effect van de bellenkolommen wordt verwaarloosd. In het eerste praktijkvoorbeeld zijn ozonprofielen bepaald met gegevens van de meestroom- en tegenstroom-kolommen van de proefinstallatie Weesperkarspel van

Waterleidingbedrijf Amsterdam en op deze gegevens is een model voor de bellenkolommen geijkt. Het model is gebaseerd op partiële differentiaalvergelijkingen die de waterstroom en de gasstroom, de overdracht van ozon van het gas naar het water en de langzame en snelle afbraak van ozon in water beschrijven. De bijdrage van de bellenkolommen in de proefinstallatie was, bij 20°C, 30% van de totale CT-waarde bij tegenstroom en 80% bij meestroom. In de praktijk is dus een hogere totale CT-waarde aanwezig dan verondersteld en derhalve een grotere desinfectie-capaciteit dan verwacht.

In het tweede praktijkvoorbeeld is de verwijdering van bentazon door aktieve koolfiters op twee locaties, drinkwaterzuivering (WTP) Rodenhuis en Reijerwaard van Hydron ZH, gemodelleerd. De aktieve koolfilters zijn geïnstalleerd in series van twee filters in een “pseudo moving bed” configuratie. Met gegevens van de proefinstallatie en het bedrijf zijn de looptijden van de aktieve koolfilters berekend en deze zijn vergeleken met de huidige bedrijfsvoering. Het model van de GAC is gebaseerd op partiële differentiaalvergelijkingen die het transport van micro-verontreinigingen door het filterbed, de overdracht van micro-verontreinigingen van het water naar de vaste fase en de accumulatie van micro-verontreinigingen in de poriën van de aktieve koolkorrels beschrijven. Het model is geijkt op gegevens van de proefinstallatie en de WTP Rodenhuis en gevalideerd aan de hand van gegevens van WTP Reijerwaard, waar de voorbelading met organisch materiaal hoger is. Verschillende scenario’s zijn geëvalueerd, waarbij uitgegaan is van een betere planning van de regeneratie van de filters en waarbij “pseudo moving bed” is vergeleken met parallelle bedrijfsvoering. Voor WTP Reijerwaard kan worden geconcludeerd dat parallelle bedrijfsvoering zal leiden tot kortere looptijden (2 jaar in plaats van 2,5 jaar), maar heeft als voordeel dat de besturing minder gecompliceerd wordt en dat het systeem een groter debiet kan behandelen. Voor WTP Rodenhuis kan worden geconcludeerd dat de huidige regeneratiepraktijk, economisch gezien, sub-optimaal is. De gemiddelde waarde van de betreffende waterkwaliteitsparameter, hier bentazon, is ver onder de toelaatbare waarde. Het aantal regeneraties van aktieve kool zou kunnen worden verminderd met 20% (1 regeneratie minder per jaar). Regeneraties zijn de belangrijkste operationele kosten van het proces en daarom kunnen aanmerkelijke economische maar ook milieuvoordelen gehaald worden als de filterlooptijd wordt verlengd.

In het derde praktijkvoorbeeld is het onthardingsproces met korrelreactoren gemodelleerd en geëvalueerd voor WTP Weesperkarspel van Waterleidingbedrijf Amsterdam, waar het water wordt onthard door natronloog te doseren. Het doel van de studie was om een optimalisatie in bedrijfsvoering te vinden door de oververzadiging van calciumionen in het gemengde product van de reactoren en de by-pass stroom te verminderen. Er zijn gegevens verzameld van één van de korrelreactoren van de WTP. Een model is ontwikkeld dat gebaseerd is op partiële differentiaalvergelijkingen die het transport van water door de reactor, de kristallisatie van calciumcarbonaat op de korrels, de groei van de korrels, het transport van de korrels door de reactor, filterbedexpansie als functie van debiet en korrelgrootte en drukval over de reactor beschrijven. Met de modelevaluaties is een verandering van de bedrijfsvoering voorgesteld om een betere waterkwaliteit (minder oververzadiging) te verkrijgen. Hiertoe zouden de deelstroomverhouding en de hoogte van het gefluïdiseerde bed moeten worden gemaximaliseerd en het debiet door de individuele reactoren moeten worden geminimaliseerd. De drukval over de reactor is in dat geval niet constant en hangt af van de watersnelheid door de reactor en de watertemperatuur. Met deze aanpak worden bij een gemiddeld debiet niet alle geïnstalleerde reactoren gebruikt. In het onthardingsproces betekent een verbetering van de productkwaliteit tevens een besparing op chemicaliën, hetgeen leidt tot een verlaging van de operationele kosten en uitstoot in het milieu. Met een verbeterde bedrijfsvoering kan de dosering van natronloog met ongeveer 5-10% worden verlaagd waardoor bijna de totale hoeveelheid zoutzuur ten behoeve van pH verlaging kan worden bespaard.

In het algemeen kan worden geconcludeerd dat dankzij de ontwikkelingen in de computerwetenschap, PC-technologie en modelleringtechnieken nieuwe mogelijkheden ontstaan die de overvloedige beschikbaarheid van gegevens gebruiken om de bedrijfsvoering van drinkwaterzuivering te verbeteren. Dit zal leiden tot een betere drinkwaterkwaliteit en/of een verlaging van de operationele kosten en/of een verlaging van de uitstoot in het milieu. Tevens wordt het inzicht in het proces verhoogd, hetgeen leidt tot meer vertrouwen in de efficiëntie van de zuiveringsinstallatie. Ingrepen kunnen worden gepland en er kan geanticipeerd worden op verstoringen. Modellering ten behoeve van de bedrijfsvoering geeft meer informatie over de status van het proces. In de praktijk kunnen niet alle parameters on-line of met regelmatige tussenpozen worden gemonitord. Goed geijkte modellen kunnen leiden tot virtuele monitoring van de productkwaliteit, resulterend in een verlaging van de analysekosten. Het gebruik van modellen om de bedrijfsvoering te evalueren kan ook leiden tot meer kennis over het proces zonder dat duur proefinstallatieonderzoek noodzakelijk is. Gebeurtenissen die nu niet worden begrepen kunnen worden geanalyseerd door gebruik te maken van gegevens uit het bedrijf. Bedrijfsvoerders worden op die manier meer betrokken bij het onderzoek, dat voortgezet kan worden in een proefinstallatie en dat kan leiden tot een alternatief zuiveringsschema. Het gebruik van modellen tijdens de bedrijfsvoering van een drinkwaterzuivering zal leiden tot een stabiel proces, waarbij snelle veranderingen in debiet, waterverdeling en dosering van chemicaliën vermeden worden. De stabiele bedrijfsvoering zal tevens leiden tot minder onregelmatigheden in het proces.

In de toekomst zullen de modellen toegepast gaan worden in de praktijk. Zij zullen worden gebruikt voor model-gebaseerde-beslissingsondersteuning en geïntegreerd worden in modelvoorspellende-“controllers” ten behoeve van on-line, geoptimaliseerde, geautomatiseerde sturing. Tevens zullen de individuele modellen aan elkaar worden gekoppeld, hetgeen resulteert in een integrale aanpak van de gehele zuiveringsinstallatie ten behoeve van een nog efficiëntere bedrijfsvoering.

LIST OF ABBREVIATIONS

CSTR	Continuous Stirred Tank Reactor
CT	Concentration times residence Time
DBP	Disinfection Byproducts
DOC	Dissolved Organic Carbon
GAC	Granular Activated Carbon
ICT	Information Communication Technology
ID	Instantaneous ozone Demand
NOM	Natural Organic Matter
ODE	Ordinary Differential Equation
PC	Personal Computer
SWTR	Surface Water Treatment Rule
TOC	Total Organic Carbon
UV	Ultraviolet light
WHO	World Health Organisation
WTP	Water Treatment Plant

LIST OF SYMBOLS

a	specific surface area (m^{-1})
A	surface area occupied by water flow (m^{2})
A_b	projected area of the bubble (m^{2})
A_g	surface area occupied by gas flow (m^{2})
A_I	interfacial area (m^{2})
$A_{I,b}$	total surface area of bubbles in the reactor (m^{2})
A_p	surface area of particle (m^{2})
A_T	total surface area of the reactor (m^{2})
$\mathrm{b}_{1,2,3}$	constants (-)
BIS	basic ionic strength (mol/m^{3})
c	(time-average component of) concentration in water (g/m^{3})
(c)	activity of compound in water (mol/m^{3})
c'	turbulent component of concentration in water (g/m^{3})
c_e	equilibrium concentration of compound in water (g/m^{3})
$c_{g,s}$	(time averaged component of) concentration in gas or solid phase (g/m^{3})
c_n	number concentration (m^{-3})
$c_{s,u}$	saturation concentration of solids in filter (g/m^{3})
C	instantaneous concentration in water (g/m^{3})
d_b	bubble diameter (m)
d_L	thickness of water film (m)
d_p	particle diameter (m)
D_{Br}	diffusion coefficient (m^{2}/s)
D_{O3}	diffusion coefficient of ozone (m^{2}/s)
D_s	surface diffusion coefficient (m^{2}/s)
D_x	dispersion coefficient in water (m^{2}/s)
$D_{x,g,s}$	dispersion coefficient in gas or solid phase(m^{2}/s)
E	activation energy (J/mol)
EC	Electrical conductivity (mS/m)
f	activity factor (-)
f_1	decay function in water
$f_{1,g,s}$	decay function in gas or solid phase
f_2	transfer function of compound from water
$f_{2,g,s}$	transfer function of compound into gas or solid phase
F	flux (g/m^{2}.s)
G	velocity gradient (s^{-1})
h	gas hold-up (-).

H	head loss (m)
I	head loss gradient (-)
IS	ionic strength (mol/m^3)
k_B	Boltzmann's constant = 1.38.10^{-23} J/K
k_d	reaction rate for direct reactions of ozone with NOM (s^{-1})
k_E	enhancement factor (-)
k_{ID}	Instantaneous ozone Demand factor (-)
k_L	transfer coefficient (m/s)
k_{O3}	slow ozone decay rate (s^{-1})
k_r	reaction rate for radical reactions of ozone with NOM (s^{-1})
k_T	kinetic constant (m^4/mol.s)
k_{UV}	decay coefficient of UV absorbance (m^3/g.s)
k_1	reaction rate ((g/m^3)$^{1-\gamma}$.s^{-1})
k_2	transfer coefficient (s^{-1})
K	Freundlich constant ((g/kg).(g/m^3)^n)
K_A	collision constant (-)
K_B	break-up constant (s)
K_D	distribution coefficient (g/m^3)$^{1-n}$
K_s	solubility constant of $CaCO_3$ (mol^2/m^6)
K_w	solubility constant of water (mol^2/m^6)
$K_{1,2}$	thermodynamic equilibrium constants (mol/m^3)
L_b	height of bed (m)
L_R	height of reactor (m)
m	m-alkalinity (mol/m^3)
M_s	mass of crystallised calcium carbonate (kg)
M_{NaOH}	molecular weight of caustic soda (kg/mol)
M_{CaCO3}	molecular weight of calcium carbonate (kg/mol)
n	constant (-)
$1/n$	Freundlich constant (-)
N_p	number of particles (-)
N_R	number of reactors in operation (-)
p	p-alkalinity (mol/m^3)
P	pressure (Pa)
q	loading of carbon grain (g/kg)
q_{max}	adsorption capacity (in g/kg)
Q	water flow (m^3/s)
Q_g	gas flow (Nm^3/s)
r	radius of particle (m)

R	universal gas constant (J/mol)
Re	Reynolds number (-)
RQ	gas to water flow ratio (Q_g/Q) (Nm^3/m^3)
T	absolute temperature (K)
$TCCP$	calcium carbonate crystallisation potential (mol/m^3)
u	time averaged component of velocity in water (m/s)
u'	turbulent component of velocity in water (m/s)
u_b	bubble rising velocity (m/s)
$u_{g,s}$	(time averaged component of) velocity of gas or solid phase through reactor (m/s)
U	instantaneous velocity (m/s)
UV	UV absorbance (254 nm) in water (m^{-1})
v_s	settling velocity of a particle (m/s)
V	volume of water (m^3)
$V_{g,s}$	volume of gas or solid (m^3)
V_p	volume of particle (m^3)
V_T	total volume of reactor (m^3)
w	weighing factor (-)
Y	yield factor (m^4/g)

α	pressure and temperature correction factor (-)
α_{pb}	adhesion efficiency (-)
β_s	surface diffusion transfer coefficient (m/s)
γ	order of reaction (-)
Δx	height of unit element (m)
ε	porosity (-)
ζ	maximum pore filling (-)
η_T	total single collector (bubble) efficiency (-)
θ	valency of ion (-)
λ_0	clean bed filtration coefficient (m^{-1})
μ	dynamic viscosity (kg/m.s)
ν	kinematic viscosity (m^2/s)
ρ_g	grain density (kg/m^3)
ρ_p	particle density (kg/m^3)
ρ_w	water density (kg/m^3)
ρ_s	density of solids (kg/m^3)
σ	surface tension (N/m)

φ_s	mass flux into grains (g/m^{2}s)
ϕ	shape factor (-)
ψ	factor accounting for initiation and scavenging of radical reactions (-)
ω	removal efficiency (-)

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EPILOGUE

It took about 10 years to come to this product. During this period I walked different dead end research pathways. This was not only instructive but sometimes also frustrating. My global mission was to find applications for modelling in drinking water treatment, using modern techniques. Drinking water treatment used (and still uses) traditional methods. Practical experience and intuition were highly appreciated and protected above all. There was a certain suspicion against a rational approach supported by computers.

In this period of time many things changed. The techniques became more and more modern. Internet developed and communication through e-mail became the standard for almost all civilians. We became inhabitants of a global village, which is small but badly protected. The dependence on computers became painfully clear with the fear for the millennium bug, which in the end did not strike as hard as we had expected. The concern about pollution and health and also terrorist attacks has led to an increased interest in the drinking water quality and the introduction of new standards. To be able to operate drinking water treatment under the new regulations it is even more necessary to ask for the support of automation and models. In this respect the privatisation fear was partly a threat to my thesis and partly a stimulus. On one hand companies were reserved to share their knowledge with others (including universities) or wanted to keep the obtained tools for themselves. On the other hand, it resulted in a benchmark procedure that stimulates the water companies to be ‘top of the class’. Every initiative that improves the position of the water company on the benchmark scale is welcomed. To be able to write the thesis it was necessary to have different types of support, which can be expressed as different wagons that together form the ongoing train.

Supervision. Hans and Johannes helped me immensely with their knowledge about the subject, the sharp analyses of theory and feed-back about the practical applicability. I am proud to have these renowned professors as supervisors in my committee.

Technological application. Without application engineering research is considered to be worthless. In the traditional drinking water world it was difficult to find companies interested in the subject. Fortunately, we found a fruitful co-operation with Amsterdam Water Supply and I am especially thankful to Karin and Eric for their help and interest.

Interaction. Exchange of knowledge and experience is important for the development of the research. Mainly in the last years I had much support from my direct research colleagues René, Patrick, Alex and Kim. Working with them is fantastic.

Multimedia. Although I am a reasonably good user of the software used, I had many questions had about modelling, use of word processors and development of Internet sites.

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Stimela. The idea was born after some Master's projects in modelling. Without the input of my colleagues of DHV consultants Stimela would never have been developed. Their contribution is invaluable.

CURRICULUM VITAE

Louis Cornelis Rietveld werd op 3 september 1961 geboren te Sint Pancras. Hij behaalde zijn VWO-diploma in 1979 te Ede. In datzelfde jaar begon hij de studie Civiele Techniek aan de Technische Hogeschool Delft. Na deze studie in 1987 aan de Technische Universiteit Delft te hebben afgerond, werkte hij tot 1991 als Bilateraal Assistent Deskundige en later als Toegevoegd Deskundige voor het Directoraat Generaal Internationale Samenwerking in Mozambique. Hij was daar werkzaam als docent/onderzoeker Gezondheidstechniek aan de Eduardo Mondlane Universiteit, Maputo.

In de periode 1991 tot 1994 had hij een aanstelling bij het Management Centrum voor Internationale Samenwerking (CICAT) van de Technische Universiteit Delft. Van 1994 tot heden werkte hij als Toegevoerd Onderzoeker en later als Universitair Docent aan de Faculteit Civiele Techniek, Departement Watermanagement, sectie Gezondheidstechniek, van de Technische Universiteit Delft.

Het promotieonderzoek werd uitgevoerd aan Technische Universiteit Delft.


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