Modelling water quality from source water to tap by integration of process models

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Abstract: The quality of drinking water delivered to the customer's tap is influenced by a number of processes; namely water treatment, disinfection and changes during transport of treated water via the distribution system. Drinking water guidelines stipulate water quality to be delivered at the customer tap. Recent studies are concerned with safe limits of chlorinated by-products, such as trihalomethanes (THM). As a result, the guideline for total THM (TTHM) in the US has been reduced to 0.08mg/L and further lowering is planned. In Australia, water utilities are examining technical feasibility of reducing TTHM and other chlorinated by-products such as haloacetic acids (HAA). To control the presence of microbial indicators (total coliform counts) a certain concentration of disinfectant is needed. Taste and odour requirements limit free chlorine concentration to less than 0.6mg/L. Analysis of the existing data suggests that the critical problem for maintaining acceptable water quality is to keep the concentration of chlorine within a certain operational window and simultaneously control concentration of disinfection by-products (TTHM and HAA). Chlorine decay, and TTHM and HAA formation, are determined by the dose of chlorine applied, and temperature, concentration and type of dissolved organic carbon (DOC) in water. DOC in treated water is influenced by the DOC concentration of source water and treatment processes applied for its reduction. The most economical and frequently used process for DOC reduction is coagulation with ferric or aluminium salts. To predict the quality of tap water a sequence of process models was developed and connected, integrating a DOC removal model, correlation of DOC and chlorine decay model parameters, a chlorine decay model, a TTHM formation model and the water transport system's hydraulics model. Such an integrated model has the capacity to predict a profile of chlorine and TTHM in the whole distribution system at any time. Possible applications of such an integrated model are also outlined including planning and operation. For example, water treatment plant optimisation, determination of compliance of chlorine operating window and maximum TTHM concentrations.

Keywords: Drinking water quality; Enhanced coagulation; Chlorine decay; TTHM; Modelling

1   INTRODUCTION

The quality of water delivered to a customer tap can be characterised by a number of parameters. The most frequently used water quality measures are:

- chlorine/chloramine
- total trihalomethanes (TTHM)
- temperature
- dissolved organic carbon (DOC)
- turbidity
- colour
- pH
- iron/manganese
- coliforms, Heterotrophic Plate Counts (HPC)
- haloacetic acids (HAA)

and a number of others.

While some water quality parameters are by their nature stable in a distribution system, others undergo substantial changes during transportation from the treatment plant to the customers via the distribution system. Examples of parameters, which undergo substantial changes include chlorine concentration, disinfection by-products and microbiological indicators.

Stable parameters can be monitored at the outlet from the plant as they do not change, but the parameters that change during the passage through the system need to be monitored at the customer's tap. It is more difficult and costly to maintain and to prove compliance of water quality parameters, which change through the distribution system. For example chlorine used as disinfectant reacts with organic matter present in water and its residual diminishes with time of travel. Therefore a sufficient dose must be applied at the treatment plant to make chlorine available at the customer's tap or, once its concentration falls too low, dosing has to be repeated (re-chlorination).

Additionally, the reaction of chlorine with organic matter present in water not only destroys chlorine, but also creates disinfection by-products (DBP) such as trihalomethanes (THM) and halo-acetic acids (HAA).

The guideline for total THM (TTHM) in the US has been reduced to 0.08mg/L and further lowering is planned (Pontius and Diamond 2000). In Australia, water utilities are examining the technical feasibility of reducing TTHM and other chlorinated by-products such as halo-acetic acids (HAA). To control microbial indicators (total coliform counts) a minimum concentration of free chlorine higher than 0.2mg/L is required. Taste and odour requirements limit free chlorine concentration to less than 0.6mg/L. Analysis of the existing data suggests that the critical problem for keeping acceptable water quality is to maintain the concentration of chlorine within a certain operational window and simultaneously controlling concentration of disinfection by-products (TTHM and HAA).

Additionally it is easy to imagine situations when it is difficult, costly or practically impossible to obtain information about water quality at the customer's tap by sampling and then benefits of modelling of water quality can be realised. For example during planning stages of treatment processes and a distribution system use of modelling may be the only way to obtain suitable data for various planning decisions which will influence water quality at customer's tap.

The sequence of events affecting water quality at the customer tap is schematically shown in Figure 1. It can be seen that there are a number of influences on the final water quality at the tap. Water authorities usually have influence on the treatment of raw water and operation of the distribution system.
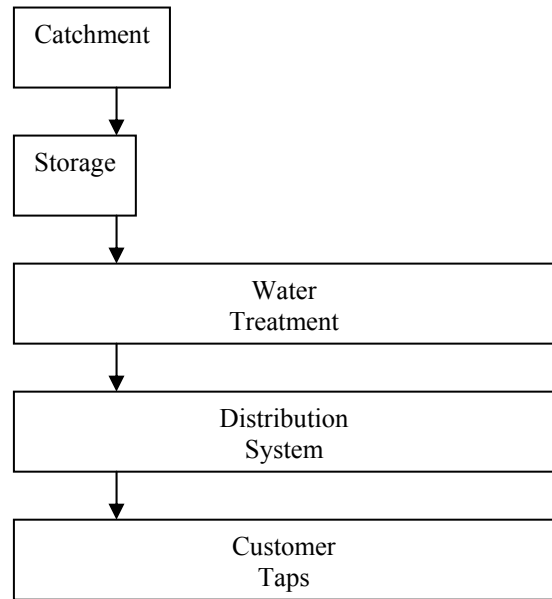
Figure 1. Schematic presentation of influences on drinking water quality

2 FORMULATION OF PROCESS MODELS

Chlorine decay and disinfection by-products formation are mainly controlled by DOC, temperature, and the age in the system. The processes that control the changes can be simplified as shown in Figure 2.
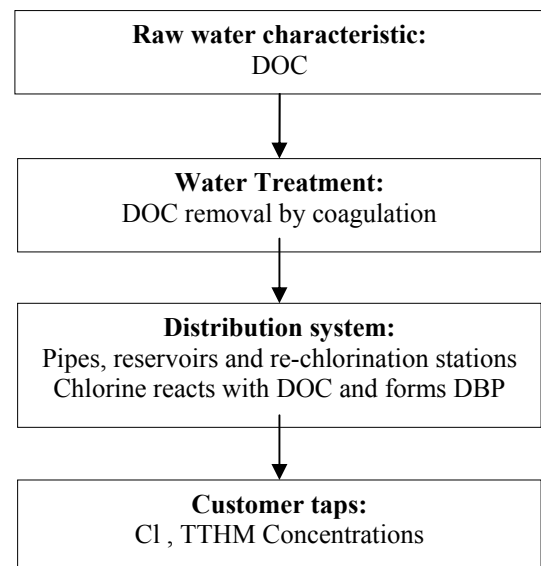
Figure 2 Simplified scheme for modelling water quality from the raw water to the tap

2.1 DOC Removal Model

Removal of DOC by enhanced coagulation is primarily affected by pH and flocculant dose. Usually more than 50% of initial DOC can be removed at low pH with sufficient coagulant dose, but there is a fraction of DOC, which is not effectively adsorbed on metal hydroxides and cannot be removed by this method. Lower pH improves DOC removal. Edwards (1997) describes DOC removal with the Langmuir adsorption isotherm where surface capacity is a polynomial function of pH:

$$\frac{c_s}{dose} = a * \frac{b*c_l}{1+b*c_l} \qquad (1)$$

and

$$a = x_1 \cdot pH + x_2 \cdot pH^2 + x_3 \cdot pH^3 \qquad (2)$$

where:

c_s is concentration of DOC adsorbed on coagulant [mg/L],
dose is coagulant dose [mg/L],
a is saturated concentration of DOC on coagulant [(mg/L)/(mg/L)],
b is saturation constant [(mg/L)$^{-1}$] and
x_1, x_2, x_3 are constants.

Kastl *et al.* (2002a) also describe DOC removal with the Langmuir isotherm but assumed different adsorption for the dissociated (A$^-$) and associated forms of humic acid (HA). Note this removes empirical dependence on pH.

$$HA \Leftrightarrow H^+ + A^- \qquad (3)$$

Humic acid represents a fraction *f* of total DOC. Then

$$[HA] + [A^-] = f * DOC^0 \qquad (4)$$

where DOC^0 is concentration of DOC in raw water.

Dissociation of humic acid is an equilibrium reaction controlled by pH:

$$K_h = \frac{[H^+]*[A^-]}{[HA]} \qquad (5)$$

and DOC is described by:

$$\frac{(DOC^0 - DOC)}{dose} = a * \frac{b*([HA] + k*[A^-])}{1 + b*([HA] + k*[A^-])}$$

$$(6)$$

where:

a and b are constants characterising the Langmuir isotherm,
k is the relative adsorption coefficient for dissociated humic acid,
K_h is the dissociation constant for humic acid and
f is the fraction of total DOC that is humic acid.

Including adsorption of non-polar compounds, which is not affected by pH, has further extended this approach. The composition of DOC in raw water is schematically shown in Figure 3, which indicates that up to 65% of DOC can be removed by a sufficient dose of coagulant at low pH.
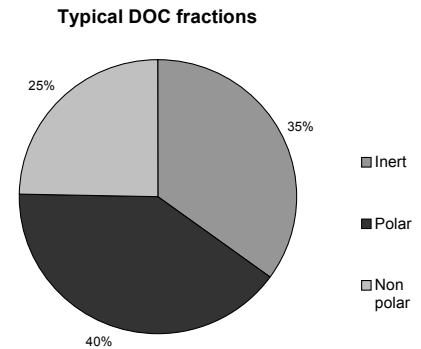
Figure 3. Typical fractions of DOC in raw water

2.2 Chlorine Decay, TTHM and HAA Formation Model

Chlorine decay in bulk drinking water is traditionally described by a first order reaction:

$$\frac{dc_{Cl}}{dt} = -k * c_{Cl} \qquad (7)$$

where c_{Cl} is chlorine concentration [mg/L] and k is the decay constant [h^{-1}].

While the chlorine decay curve has this approximate shape for a selected dose, a single value of the decay constant k cannot describe decay for various initial concentrations. A model proposed by Kastl *et al.* (1999) describes chlorine decay kinetics for various initial chlorine doses and temperatures in the water phase. This model can also describe the concentration of free and combined chlorine with time. This distinction is very important at the end of the distribution system, where free chlorine constitutes a lower percentage of total chlorine concentration, but still determines disinfection efficiency.

In this model, it is assumed that there are two groups of organic compounds: fast reacting and slow reacting. These organic groups are again subdivided into two to account for free and combined chlorine. The new subdivision results in four types of organic compounds being considered:

- Fast reacting organic compounds (FRA)

- Slow reacting organic compounds (SRA)

- Fast reacting organic-nitrogen compounds (FNA)

- Slow reacting organic-nitrogen compounds (SNA)

Based on these assumptions the following reaction scheme is proposed:

FRA +Cl-> Cl⁻ + αTTHM

SRA +Cl-> Cl⁻ + αTTHM

FNA +Cl-> CCl

SNA +Cl-> CCl

CCl   -> Cl⁻ (8)
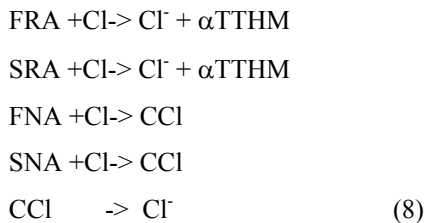
where Cl and CCl are the free and combined chlorine concentrations, TTHM is concentration of total trihalomethanes and α is yield of TTHM per mg of chlorine reacted.

Five reaction constants, four initial concentrations and activation energy (E) describe the system. The value of E is assumed to be universal for all reactions. This method of description is independent of initial chlorine dose and temperature. Laboratory experiments monitor concentrations of free and total chlorine and TTHM (over extended period), after dosing water with different initial chlorine concentrations. The model constants are fitted to the experimental data. The advantage of this approach is that it links chlorine decay and TTHM formation. Interestingly the yield of α TTHM (amount of TTHM generated per unit of chlorine reacted) is constant across a wide range of treated DOC concentrations.

The effect of temperature can be described by Arrhenius' equation assuming that all reactions have the same activation energy:

$$k_t = k_{20} * \exp(\frac{E/R}{(273+20)*(273+t)} * (t-20)) \qquad (9)$$

where:
k_t and k_{20} are reaction constants at temperature t and 20°C respectively and
E/R is activation energy over universal gas constant [K].

The above set of equations describes chlorine decay and TTHM formation in bulk drinking water. HAA formation is similar to TTHM, ie. there is a certain yield of HAA generated per unit of chlorine reacted. However, yield of HAA is not constant, as is TTHM yield, but decreases with DOC removal. The more DOC removed, the less HAA is formed per unit of chlorine reacted. This characteristic makes HAA much easier to control than TTHM. This is because TTHM production is only reduced through reduction in chlorine consumption, whereas HAA production is reduced due to reduction in chlorine consumption reduction and in yield per unit of chlorine reacted.

2.3 Link between DOC and chlorine decay

The enhanced coagulation model above describes the resulting DOC as a function of coagulant type, dose and pH. DOC remaining in the water is still composed of a number of fractions from the point of view of chlorine decay. Namely it has to be determined how DOC removal changes

concentrations of FRA and SRA in the chlorine decay model.

Results of experiments indicate that enhanced coagulation is more "selective" to remove SRA than FRA. Therefore better coagulation treatment significantly improves chlorine stability in the distribution system after the fast initial decay.

The relationship of reduction of initial FRA and SRA is approximately linear with different slopes.

$$FRA^0 = FRA^R - k_F*(DOC^R-DOC)$$

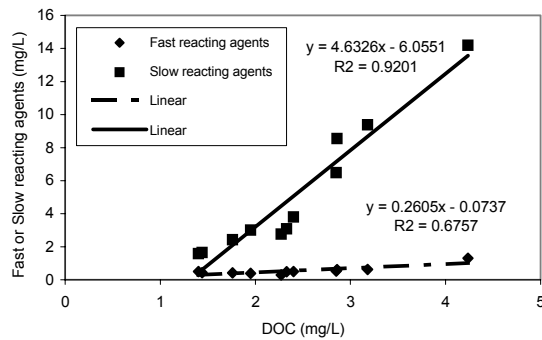$$SRA^0 = SRA^R - k_S*(DOC^R-DOC) \qquad (10)$$

where:
superscript 0 indicates initial concentrations of fast and slow reacting agents used in the chlorine decay model,
superscript R indicates Raw Water,
DOC indicates DOC in treated water and
k_F , k_S are constants of proportionality between concentrations of DOC and chlorine decay compounds.

Figure 4. Relationship between DOC removal and Chlorine decay parameters

Figure 4 shows how concentrations of fast and slow reacting compounds in chlorine decay model are affected by DOC removal. It can be seen that removal of DOC has much more pronounced effect on reduction of slow reacting compound than on fast reacting. This is consistent with a theory that slow reacting compounds are high molecular weight humic acids, which are easier to remove than low molecular weight fast reacting compounds.

3   INTEGRATION OF PROCESS MODELS INTO DRINKING WATER DISTRIBUTION SYSTEM QUALITY MODEL

The above water quality models, such as chlorine decay and TTHM formation models can be coupled with a hydraulic model of a drinking water distribution network. Details of

implementation of the above models within the EPANET software are described by Kastl *et al.* (2002).

Quality processes taking place in bulk water, such as chlorine decay and TTHM formation, are also accelerated by wall material or biofilm on the pipe surface. The concept of equivalent diameter is a convenient way of linking wall reaction with bulk reaction, when they are related, as in the case of biofilm formation. Then:

$$r_t = r_b * (1 + \frac{d_e}{d}) \qquad (11)$$

where:

r_t and r_b are total (including the surface) and bulk reaction rates respectively,
d is pipe diameter and
d_e is the 'equivalent diameter' constant, characterising the reaction rate on the surface relative to the bulk water rate.

In the case of reaction with the pipe material itself, an independent wall reaction rate is suitable, as applied in EPANET.

## 4   APPLICATIONS OF SOURCE WATER TO CUSTOMER TAP DRINKING WATER QUALITY MODEL

Modelling of water quality changes from raw water to customer tap has numerous applications for the water industry. It can be used for operational support for selecting a suitable chlorine dose or set points at rechlorination stations and as a powerful planning tool for combined optimisation of a proposed water treatment plant and a drinking water distribution system.

A specific application may be optimisation of an compliance of chlorine within acceptable operation window (for example minimum 0.2mg/L and maximum of 0.6mg/L) and TTHM below a specified level (for example 0.08 mg/L).

Figures 5 and 6 show examples of chlorine and TTHM profiles through a distribution system at a given time.
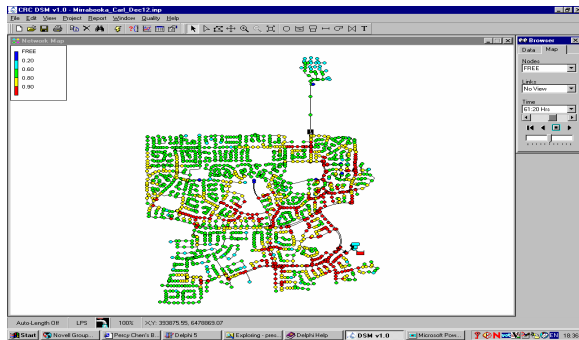
Figure 5. Free chlorine profile in a distribution system.
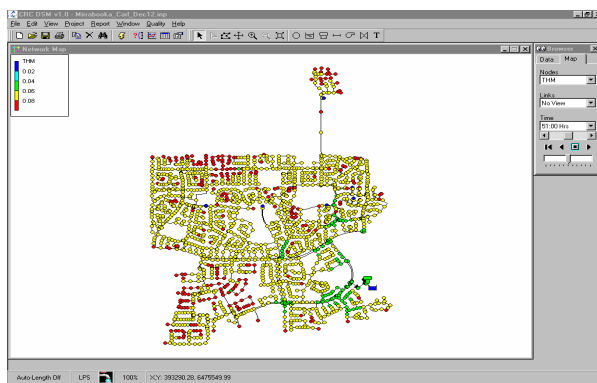
Figure 6. TTHM profile in a distribution system

5   CONCLUSIONS

Water quality modules developed by Sydney Water Corporation and the Cooperative Research Centre for Water Quality and Treatment are suitable for integration with a hydraulic model to provide substantial capability of water quality modelling.   In a demonstration project the modules of chlorine decay, TTHMs formation and effects of biofilm were "added" to EPANET network model.

This model has a potential to be used in numerous applications considering water quality in a drinking water distribution system from planning to operation.

7   REFERENCES

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