Water quality decay modelling in hydraulic pressure systems

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Abstract A mathematical model able to evaluate water quality variations in complex hydraulic pressure systems has been developed. The model consists of a set of mass balance equations for tanks, pipes and nodes. It has been applied to predict chlorine concentration inside a case-study water network described in literature by using different expressions of chlorine decay coefficients, obtained in laboratory tests and expressed as a function of the residence time of water in pipes, the initial chlorine concentration, the history and temperature of water. The results showed little variations of the chlorine concentrations and the need to calibrate the parameters of chlorine decay coefficients expressions on full scale hydraulic systems.

Keywords Chlorine decay; water distribution systems; water quality modelling

Introduction
Recently, many mathematical models have been proposed to simulate water quality parameters variations inside hydraulic networks. The models differ for the flow conditions and the phenomena considered and also for the nature of the examined substances. Most of the models refer to steady-state conditions (Elmaalouf, 1992; Shah and Sinai, 1988) and consider only the advective transport of substances in the pipes, while the diffusion phenomena are ignored (Liou and Kroon, 1987; Murphy, 1985; Wood and Ormsbee, 1989). Moreover, it is usual to distinguish the conservative substances from the non-conservative ones. Inside the system, the change of concentration of the conservative substances is exclusively due to flows mixing in each node. For the non-conservative substances the variations are induced also by reactions and decay phenomena in the pipes and tanks located along the system. Some of the proposed mathematical models deal with conservative substances (Elmaalouf and Kim, 1997). Others models refer to non-conservative ones (Liou and Kroon, 1987; Maione et al., 1991; Odzemir and Ger, 1998; Rossman et al., 1994), and particularly to chlorine, whose high reactivity determines its decay in hydraulic systems. The wide use of chlorine as a disinfectant is mainly because it is relatively cheap, easy to use, effective in limiting micro-organism growth, and persistent inside the pipelines of the hydraulic system. Nevertheless, chlorine causes serious problems both to the system structure and water quality, because of its residual concentration and DBPs production. In recent years these problems have been aggravated either by the gradual increase in use of low quality water or the necessity to supply networks with flows with very different physical–chemical characteristics, whose mixing can favour the above-mentioned alterations.

Mathematical modelling of processes influencing water quality changes in distribution systems is usually based on a two-step approach. First, using a hydraulic one-dimensional model able to take into account the real behaviour of the system, hydraulic parameters are evaluated, such as flow velocities in pipes, water levels in reservoirs, piezometric heads on nodes and discharges flowing in or out from the nodes. Secondly, starting from these values, water quality parameters are evaluated using a water quality sub-module, together with their changes due to mixing, decay reactions and hydrodynamic phenomena.
Also many expressions of the chlorine decay have been proposed, empirically or semi-empirically. The simplest one is the first order decay model, in which the chlorine is assumed to decay exponentially. More complex relationships consider the chlorine decay as a function of chemical and physical properties of water.

In the first part of the paper the proposed mathematical model is described (Pianese et al., 1995, 1997a, 1997b). The model differs from the existing ones because it is more complete, has shorter processing times and makes possible the adoption of physically based criteria that allow to follow the development of each single process within the network. The model is able to evaluate the changes in time and space of the characteristics of the water flowing through a complex water distribution system compose of free water surface tanks, pumping stations, and pipes connecting the tanks one to another, bringing the water to the delivery nodes. In the second part of the paper, using different expressions of chlorine decay model, the mathematical model is applied to a case-study hydraulic network, in order to evaluate the variations of the chlorine concentrations values.

**Mathematical model**

The proposed model is based on a two step approach. It evaluates the variations of a generic substance inside the hydraulic system due to the following phenomena: (i) water mixing on the nodes of the system (tanks and pipes junctions); (ii) advection; (iii) dispersion; (iv) molecular diffusion; and (v) reaction. The water quality sub-module consists of mass balance equations able to explain the variations of the substances present:

- In the water contained into the tanks existing in the system.

\[
C_t \bigg| \begin{array}{l}
\left[ V_v C_{t-\Delta t} \right]_v + \Delta t \sum_{n=1}^{N_v} Q(n,j)C|_{t=L} + \Delta t \cdot M_v - S_v \\
V_v + \Delta t \sum_{z=1}^{N_v} Q(j,z) + \Delta t Q_{str}
\end{array}
\]

- In the water flowing thorough the nodes.

\[
C_j = \frac{\sum_{n=1}^{N_j} Q(n,j)C_n + M_j}{\sum_{z=1}^{N_j} Q(j,z) + Q_o(j)}
\]

- In each elementary cell in which the volume of water contained in each pipe is divided (see below).

\[
\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial s} + D_T \frac{\partial^2 C}{\partial s^2} + D_M \frac{\partial^2 C}{\partial s^2} - S_p
\]

where \( C \) = generic substance concentration at instant \( t \) and abscissa \( s \); \( U \) = flow velocity; \( D_T \) and \( D_M \) = eddy and molecular diffusion coefficients; \( S_v \) and \( S_p \) = reactions terms in tanks and pipes; \( N_{j1} \) and \( N_{j2} \) = number of pipes, respectively, inflowing and outflowing from the node \( j \); \( Q(n,j) \) = flow from node \( n \) to node \( j \) \((n=1, 2, \ldots, N_{j1})\); \( C_n \) = concentration at the terminal section of the pipe connecting nodes \( n \) and \( j \); \( M_j \) = mass directly flowing into node \( j \) and the tank \( v \); \( Q(j,z) \) = water discharge flowing from node \( j \) towards nodes \( z \), hydraulically located downstream \((z=1, 2, \ldots, N_{j2})\); \( \Delta t \) = calculus time interval; \( Q_o(j) \) = flow distributed to the users at the node \( j \); \( V_v \) = mean water volume in the tank \( V \) during \( \Delta t \); \( C_{t-\Delta t} \bigg|_V \) = concentration in the tank at and \( t - \Delta t \); \( Q_{str} \) = discharge flowing from the tank spillway; \( C|_{s=L} \) = concentration in the last node of the pipe with flow entering the tank; \( M_v \) = mass introduced into the tank \( V \).
The solution technique used in order to take the advection phenomena into account is based on a Lagrangian approach, in which the water volumes flowing through the different pipes are subdivided into cells which are traced as they move within the pipes. In practice, this approach considers, for each flow condition, the subdivision of the water volume present in each pipe with length $L_y$ into a number of segments $P_y$ (elementary cells). Generally speaking, $P_y$ varies from one pipe to another; for the same pipe, if the flow is not strictly in steady-state conditions, it also varies time after time. Then, the position of each cell is traced starting from the moment in which the cell itself comes into the pipe until the moment it leaves the pipes. For each pipe, if $U_y$ is the mean flow velocity, the number of subdivisions $P_y$ will have to respect the following condition:

$$P_y = \frac{L_y}{\Delta t U_y} \quad \text{with} \quad y = 1, 2, ..., R$$

(4)

where $R$ is the number of pipes in the network.

Nevertheless, as it is generally impossible to respect Eq. (4) for all the network pipes at the same time, it will be sufficient to obtain only an approximate equality:

$$\forall y, \quad P_y \equiv \frac{L_y}{\Delta t U_y} \quad \leftrightarrow \quad \forall y, \quad \left| \frac{L_y}{\Delta t U_y P_y} - 1 \right| \leq \varepsilon$$

(5)

with a small value of $\varepsilon$ (for example, $\varepsilon = 0.01–0.05$).

The Lagrangian approach makes it possible to solve, for each cell, instead of the previous pipe transport Eq. (3), the following equation:

$$\frac{\partial C}{\partial t} = D_l \frac{\partial^2 C}{\partial s^2} + D_M \frac{\partial^2 C}{\partial s^2} - S_p$$

(3')

The proposed approach allows us to go beyond some limitations of the most popular water quality model used on hydraulic networks, named EPANET (Rosmann et al., 1994). EPANET consists of a set of equation equal to Eqs (1)–(3), solved by means of a Lagrangian approach too. However, EPANET considers that the length of each cell is equal to the length of the pipe with the shortest travel-time ($L_{min}$) whereas the number of cells of each pipe is equal to the ratio between its length ($L_y$) and $L_{min}$. This option may cause severe faults, because the mass of a generic substance coming to each node from confluent pipes is not well modelled and also because the lengths of the pipes that are considered in the calculations can considerably differ from the actual ones.

**Chlorine decay models**

The reaction terms in Eqs (1) and (3), $S_y$ and $S_p$, depend on the substance considered and on the phenomena modelled. The most interesting technical case is relative to the modelling of the chlorine content. Chlorine is known to be consumed both in the bulk liquid (bulk decay) and at the wall of the pipes and tanks (wall decay). The first is related to the chlorine reactions with inorganic and organic substances, naturally present in the water source; the second is due to the reaction, at the inner wall’s of pipes and tanks, with sediments and biofilms and, exclusively for metallic pipes and tanks, also with pipes material and corrosion products. The bulk decay is always modelled using a one-dimensional approach and represented by the following first-order equation:

$$S_b = -K_b C$$

(6)

where: $S_b = S_y$ or $S_p$ for tanks and pipes, respectively, and $K_b =$ bulk decay coefficient.

Eq. (6) generally has been used with a constant value of the bulk decay coefficient (Rossmann et al., 1994), whereas recently published papers relate the chlorine decay with water temperature, initial chlorine concentration ($C_o$) and a eventual addition of a
disinfectant (also chlorine) in the water. The decay coefficient $K_b$ is inversely proportional to $C_o$ and directly proportional to the temperature $T$. For a known value of $T$ and three different types of water, Fang Hua et al. (1999) proposed the following experimental expression correlating $K_b$ and $C_o$ (with $K_b$ and $C_o$ in units of h$^{-1}$ and mg l$^{-1}$ respectively), valid for chlorine concentration ranging from 0.11 to 0.52 mg l$^{-1}$:

$$K_b = 0.018 / C_o - 0.024$$  \hspace{1cm} (7)

On the basis of the same experimental tests, Fang Hua et al. (1999) also proposed the following exponential expression correlating the bulk decay coefficient with the temperature:

$$K_b C_o = ae^{bT}$$  \hspace{1cm} (8)

where $a$ and $b$ depend on the type of water examined; 0.0098 and 0.0512, respectively, for water taken from a tap at the University of Birmingham; 0.0029 and 0.112 for a rechlorinated solution, composed by distilled water and humic acid; 0.005 and 0.0841 for the water sample taken at the final point of the Frankley Water Treatment Works.

The decay at the wall is related to the chlorine interaction with pipes materials (corrosion), deposits and biofilms. The corrosion phenomenon could be remarkable only for metallic pipes. Chlorine consumption occurs both at the metal/electrolyte interface (electrochemical consumption) and in the bulk liquid (chemical consumption) induced by its reaction with ferrous ions produced by iron dissolution. Frateur et al. (1999) showed that the chlorine chemical consumption is prevalent. Its decay rate is expressed by the following equation:

$$S_{cor} = (M_{Cl_2} / Fd) \times i_{cor}$$  \hspace{1cm} (9)

where $S_{cor}$ is the reaction rate term caused by corrosion; $M_{Cl_2}$ is the Cl$_2$ molar weight (70.9 g mol$^{-1}$); $F$ is the Faraday’s constant (96487 C mol$^{-1}$); $d$ is the pipe diameter; $i_{cor}$ is the corrosion current density (A m$^{-2}$).

The production of loose deposits on the pipes of hydraulic systems is another cause of chlorine decay. Generally, these deposits own a high percentage of organic content, capable of stimulating the development of microorganisms as bacteria and bacterial predator. They also give rise to a high chlorine demand, specially in the case of a resuspension. Chlorine decay due to loose sediments is assimilated by the bulk decay and modelled with a first order equation (Gauthier et al., 1999), equal to Eq. (6). The value of the decay constant ($K_d$) depends on the organic carbon and the nitrogen concentrations and it can also be greater than $K_b$.

Another phenomena to consider on decay chlorine modelling in hydraulic systems is the development of biofilms on the internal walls of the pipes, particularly in the case of not negligible concentrations of carbon contents [greater than 0.6 g m$^{-3}$ of biological dissolved organic carbon (BDOC)]. As in the previous case, chlorine decay related to biofilms is usually modelled with a first-order equation. The decay coefficient value ($K_{bio}$) depends on the water composition and pipes inner wall conditions; it is assumed to be higher for small pipe diameters ($d < 40$ mm) and not negligible BDOC (Lu et al., 1999).

All the models mentioned above adopt a one-dimensional approach. Just a few models have been proposed by simulating the phenomena using a two-dimensional approach. Rossman et al. (1994) used a film resistance model of mass transfer to model the chlorine decay at sites along the pipe wall. The proposed equation is:

$$S_w = \frac{4K_w S_h D_M}{d^2 K_w + dS_h D_M} \times C$$  \hspace{1cm} (10)
where \( S_w \) = global wall reactions terms in pipes; \( K_w \) = wall decay coefficient with unit of length over time; and \( S_h \) = Sherwood number.

Ozdemir and Ger (1998) proposed a two-dimensional steady-state model to simulate both chlorine disappearance mechanism (axial convection and radial diffusion) under turbulent, transitional and laminar flow regimes using realistic velocity profile, and variability of decay constants along the pipes. They introduced and calibrated a correction factor (\( F_c \)) to convert one-dimensional model solutions (\( C_{1D} \)) into more refined concentrations, obtainable by using a two-dimensional approach (\( C_{2D} \)):

\[
C_{2D} = C_{1D} / (1 + F_c)
\]  

(11)

with \( F_c \) given by:

\[
F_c = 0.72677 W_d L_y / \nu Re^{0.9538}
\]  

(12)

where \( \nu \) = the kinematic viscosity of water; \( W_d \) = chlorine consumption rate at the pipe wall, assumed by authors equal to \( 1.0 \times 10^{-6} \) m s\(^{-1} \); \( Re \) = Reynolds number (\( = U_y d_y / \nu \)).

The results obtained by Ozdemir and Ger demonstrate that chlorine decay rate in pipes and tanks of hydraulic systems is strictly related to hydrodynamic conditions; it increases as the flow regime becomes transitional and then laminar. This is caused by the increase of chlorine consumption at the wall’s pipe corresponding to a high value of the residence time of the water on the system. Under normal conditions, the residence time is very high in many points of the system, since sizes of the secondary pipes of the distribution system are chosen accordingly to the emergency fire demands and thus their velocities are usually very slow. In these conditions, dispersion and molecular diffusion of the chlorine inside the pipes are not negligible. They are accurately considered in the mathematical model described in the previous paragraph (Pianese et al., 1995, 1997a,b), whereas they are overlooked by most of the remaining ones.

### Model application

The model described in the previous paragraph has been applied to the water network described by Elmaalouf (1992) and already examined in a previous work (Pianese et al., 1997). The network is schematically shown in Figure 1, where the geometric features are also reported. The system is fed by two pumping stations located in nodes 9 and 10, which draw the necessary flows from constant level tanks with height (referred to a datum) respectively of 6.10 m and 3.05 m and both with chlorine concentration of 0.4 mg l\(^{-1} \). The water outflows through the four nodes, characterised by discharges equal to 113.49 l s\(^{-1} \) (node 8), 141.86 l s\(^{-1} \) (node 5) and 283.72 l s\(^{-1} \) (nodes 3 and 4), whereas \( \nu \) is assumed equal to \( 1.14 \times 10^{-6} \) m\(^2\) s\(^{-1} \). The roughness formula used to test the hydraulic sub-module is that of Hazen–Williams with the coefficient \( C_{H-W} = 120 \). The mean velocity value in each pipe is reported in the table of the Figure 1.

The mathematical model has been repeatedly applied in order to evaluate the variations in the chlorine concentration values corresponding to some of the reaction formulas described in the previous paragraph. The calculations have been carried out with a maximum error (\( \varepsilon \)) lower than 5% (it has been calculated as \( \varepsilon = 0.0499 \)). Consequently, taking a calculation time interval lower than one minute (\( \Delta t = 54.32 \) s), the number of cells obtained for the different network sections turned out to vary from a minimum of 4 to a maximum of 140. In order to consider the effects due to dispersion and diffusion phenomena, \( D_T \) and \( D_M \) have been calculated \( D_T = 4 \times 10^{-3} \) m\(^2\) s\(^{-1} \) and \( D_M = 0.5 \times 10^{-9} \) m\(^2\) s\(^{-1} \). Seven different scenarios have been examined, whose results are summarised in Table 1. In the first scenario, chlorine concentration in each node of the network has been calculated neglecting the wall reaction terms and considering in all the pipes a constant value of bulk
decay coefficient, equal to 0.504 day\(^{-1}\); this value of \(K_b\) corresponds to the value obtained from Eq. (7) with \(C_o = 0.4\) mg l\(^{-1}\) (equal to the chlorine concentration inside the tanks). In the second scenario the reaction at the walls of pipes has been neglected too, but the bulk decay coefficient has been assumed variable with Eq. (7), in order to consider the chlorine consumption inside each pipe. As it can be verified (see above Eq. (8) and Table 2 of the paper of Fang Hua \textit{et al.}, 1999), the calculated values of the chlorine concentrations related to the second scenario correspond to the case of the water sample taken at the final point of the Frankley Water Treatment Works with a temperature of 6°C. Supposing that the same water is rechlorinated, in the third scenario the coefficients \(a\) and \(b\) of Eq. (8) have been assumed equal to 0.0029 and 0.112, respectively. The fourth scenario considers that the temperature of the rechlorinated water is 15°C, so to evaluate the effect of the temperature on the bulk decay. In the fifth scenario the correction factor \((F_c)\) proposed by Ozdemir and Ger (1998) has been applied to the one-dimensional model solutions.

As can be observed from the results reported in the Table 1, for scenarios 1–5 the chlorine concentrations values in each node are almost the same. The model gives results certainly congruent: for scenarios 2 and 3 the concentrations are lower than that evaluated for scenario 1, because the bulk reaction rate increases when the chlorine concentration itself is decreasing (Eq. (7)) In the case of rechlorinated water a temperature increase gives rise to higher chlorine decay, as can be observed analysing results of scenarios 3 and 4; the wall chlorine consumption contributes to reduce its concentration inside the network, as deduced comparing the data for scenarios 1 and 5. However, the formulas used to model the reaction phenomena inside the pipes seemed to be poorly effective, probably because they have been obtained by mean laboratory tests, without the calibration on real systems. This result is also confirmed for scenario 6 related to the case of a network differing from the one represented in Figure 1, only for the bigger diameters of the pipes, looking forward to verify the effect of the correction factor \((F_c)\) with lower velocities. In particular, the scenario is referred to the case of the following values of the diameters: pipes 1, 7 and 13, \(d = 1,000\)
pipes 2, 3, 4, 6, 9 and 12, \( d = 800 \) mm; pipes 5, 8, 10 and 11, \( d = 500 \) mm, with corresponding velocities comprise between 0.072 and 1.525 m s\(^{-1}\). Chlorine concentrations are lower than the ones related to scenario 5, although they are very close. The use of a global decay reaction term obtained from experimentally tests on a real network is expressed by Eq. (10), whose application with \( K_w = 0.15 \) m day\(^{-1}\) (Rossman \textit{et al.}, 1994) has given rise to chlorine concentrations calculated for scenario 7. As it can be seen, the chlorine concentration decreases inside the pipes, with big differences between the values calculated in each node even in steady-state conditions.

To evaluate the results of the proposed chlorine consumption models even in unsteady conditions, the case has been considered in which the water distribution system shown in Figure 1, under operating conditions as enumerated above, is subjected to a sudden dose of chlorine into the two tanks. It has been assumed that the chlorine is introduced into both tanks almost simultaneously. In particular, the following inlet law is considered for tank 9 (\( t \) in seconds and \( M_C \) in mg s\(^{-1}\)): \( t = 0 \rightarrow M_C = 50.00; t = 3,600 \rightarrow M_C = 99.24; t = 5,400 \rightarrow M_C = 99.24; t = 7,200 \rightarrow M_C = 50.00; t = 86,400 \rightarrow M_C = 20.00. \) Chlorine is introduced into the tank located in the node 10 according to the following law: \( t = 0 \rightarrow M_C = 90.00; t = 1,800 \rightarrow M_C = 150.00; t = 3,600 \rightarrow M_C = 229.88; t = 5,400 \rightarrow M_C = 229.88; t = 86,400 \rightarrow M_C = 50.00. \) The results of the model related to node 4 and obtained in the conditions of the previous scenarios 1, 2, 3 and 7 are shown in Figure 2. Examination of various curves clearly shows that the model can simulate chlorine concentrations changes due to variable inlet. However, the different phenomena taken into account by Eqs (6), (7), (8) and (9) seems to have a very little influence on the chlorine concentrations decrease. The congruent trend of the results is again confirmed. For example, comparing the results of the scenarios 1 and 2, it is possible to note that the curves opened wide as the chlorine concentration decreased.

**Table 1** Chlorine concentration (mg l\(^{-1}\)) for the various scenarios

<table>
<thead>
<tr>
<th>Node</th>
<th>Scenario 1</th>
<th>Scenario 2</th>
<th>Scenario 3</th>
<th>Scenario 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.39863</td>
<td>0.39799</td>
<td>0.39742</td>
<td>0.39619</td>
</tr>
<tr>
<td>2</td>
<td>0.39863</td>
<td>0.39798</td>
<td>0.39741</td>
<td>0.39613</td>
</tr>
<tr>
<td>3</td>
<td>0.39908</td>
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<td>0.39739</td>
</tr>
<tr>
<td>4</td>
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<td>0.39626</td>
<td>0.39519</td>
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</tr>
<tr>
<td>5</td>
<td>0.39809</td>
<td>0.39709</td>
<td>0.39610</td>
<td>0.39394</td>
</tr>
<tr>
<td>6</td>
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<td>0.39587</td>
<td>0.39118</td>
<td>0.38785</td>
</tr>
<tr>
<td>7</td>
<td>0.38170</td>
<td>0.32675</td>
<td>0.29632</td>
<td>0.28896</td>
</tr>
</tbody>
</table>

**Figure 2** Chlorine concentrations trend in node 4 in different scenarios
Conclusion
The changes in the quality characteristics of water flowing in a water distribution system are very often evaluated considering a number of processes, such as mixing, decay and reactions with the substances contained in the water or present on the pipe’s internal wall. Recently a number of papers have been published in which the influences on the decay rate of chlorine concentrations due to different phenomena have been highlighted and evaluated: chlorine initial concentration, water temperature, history and residence time of the water, etc. In order to evaluate the influences of these phenomena, a proposed mathematical model has been applied, with some variations considering the different processes that can happen as consequence of the above factors. The tests carried out, showed that, generally speaking, the influence of the chlorine initial concentration, water temperature and history and also of the Reynolds number (in the typical range that corresponds to the pipes of the hydraulic network) are almost negligible, probably, because of the expression proposed in literature, that are no more calibrated on real networks.

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