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Residual chlorine in the extremities of the drinking water distribution system: the influence of stochastic water demands

M. Blokker[a]*, J. Vreeburg[a,b], V. Speight[c]

[a] *KWR Watercycle Research Insititute, Groningenhaven 7, 3430 BB Nieuewegein, the Netherlands;*
[b] *Wageningen University and Research Centre, Wageningen, the Netherlands;*
[c] *Latis Associates, Arlington, VA, USA*

Abstract

An all pipes network model with stochastic drinking water demand patterns (bottom-up) was used to study the difference in residual chlorine predictions compared to a transport model with one demand pattern (top-down). The results showed that the demand model had a small effect in combination with bulk decay at constant temperature. The top-down model results in higher chlorine predictions, but not at all locations and not consistently throughout the day. Including wall decay is important but only at certain locations. The bottom-up approach can help clarify the residence time at the worst locations.

Keywords: Chlorine residual; stochastic modelling; drinking water demand modelling

1. Introduction

In many countries, it is a regulatory requirement for secondary disinfection of drinking water distribution systems (DWDS) to maintain a detectable chlorine residual from system entry to its farthest extremities. Because of losses in the network, a much higher concentration of chlorine at entry is needed to achieve a detectable concentration at the DWDS extremities. High chlorine concentrations at the point of entry may lead to taste and odour problems or disinfection by-products that are harmful to human health. The goal is to minimize the amount

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* Corresponding author. Tel.: +31-30-6069533; fax: +31-30-6061165.
E-mail address: mirjam.blokker@kwrwater.nl

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of chlorine dosed, while still achieving microbial control and meeting requirements for chlorine residual throughout the DWDS.

Chlorine is lost by reaction with substances left in the water after treatment, particularly organic matter and inorganic substances such as iron, manganese or ammonia. Chlorine decay thus depends on the residence time (Vasconcelos et al. 1997). Especially in the extremities of the DWDS, residence times can be much longer than the simple transport model would suggest (Blokker et al. 2010a). A detailed all pipes hydraulic network model with stochastic drinking water demand patterns (bottom-up model) will lead to different residual chlorine levels than a transport model with one specific demand pattern (top-down model). The chlorine decay coefficients also depend on flow velocity in Cast Iron (CI) pipe networks (Clark et al. 2010) and on temperature (Fisher et al. 2012). The temperature in the DWDS depends on the soil temperature, flow velocities and residence times in the DWDS (Blokker and Pieterse-Quirijns 2013).

Software packages for simulating flows in complex DWDS, commonly used to assess the system hydraulic performance, include simple chlorine decay models (Rossman 2000). For assisting a water company to achieve secondary disinfection goals, an accurate chlorine decay model is required. However, site-specific model parameters are required so there is a need for model calibration (Fisher et al. 2012). EPANET MSX (Shang and Uber 2008) allows for incorporating more complicated decay models, which include dependence on temperature, residence time and flow velocity. With these detailed descriptions of the chlorine decay model, the actual residence time, wall contact and flow velocities should also be described on this level. The bottom up approach for demand modelling offers good opportunities for this (Blokker et al. 2010a).

To study the effect of the bottom up approach versus the top-down approach on chlorine residuals we applied various chlorine decay models in a bottom-up and top-down model of an actual DWDS.

2. Methods and Materials

2.1. Residual chlorine model

For systems using free chlorine, the water leaving the treatment plant typically has an initial chlorine concentration of 1.0 – 1.5 mg/L. Chlorine decay can be modelled with several levels f detail. The most commonly used chlorine bulk decay model is a first order reaction (Vasconcelos et al. 1997):

$$\frac{dC_{Cl}}{dt} = -k_T \cdot C_{Cl} \tag{1}$$

where C_{Cl} is the concentration of free chlorine (mgCl/L). While several studies have demonstrated that a second-order reaction can provide a more accurate prediction of chlorine concentrations (Boccelli et al. 2003; Clark 1998; Fisher et al. 2012; Speight et al. 2009); these models require an estimation of the concentration of reactant material. For this study a simplified first-order bulk chlorine decay model was selected to focus on the impact of demand modelling, temperature and wall reactions. The selection and parameterization of an appropriate bulk chlorine decay model would further influence the chlorine predictions but was beyond the scope of this study.

Several first-order chlorine bulk decay values are reported in the literature: from 0.12 to 17.7 $\mathrm{L.mg^{-1}.day^{-1}}$ (DiGiano et al. 2000; Fisher et al. 2012; Rossman et al. 2001; Vasconcelos and Boulos 1996; Vasconcelos et al. 1997) at temperatures ranging from 14 to 28 °C. There are many other studies that have looked at calibration of coefficients, the ones we present are just examples. In Eq. (1), k_T is the reaction rate coefficient (L/mgCl/h) which depends on the temperature of the water T_{water} (ºC):

$$k_T = k_{20} \cdot \exp\left(\frac{-E/R \cdot (20 - T_{water})}{(273+20) \cdot (273 + T_{water})} \right) \tag{2}$$

with *E/R* the activation coefficient (K) where an *E/R* equal to 12,104 and 6,154 means doubling of the decay rate at T = 25 ºC respectively T = 30 ºC. Here, k_{20} the base value at a reference temperature of 20 ºC. For this study we selected k_{20} equal to 0.87 L.mg^{-1}.day^{-1}, which is approximately the median value from the literature data. With a chlorine level of 1 mg.L^{-1} at the entry point and a maximum residence time of 48 hours, a bulk water reaction rate coefficient of 0.87 L.mg^{-1}.day^{-1} will ensure a minimum target level of 0.2 mg.L^{-1} at the customers' taps in the absence of wall decay reactions.

Clark et al. (2012) have derived a chlorine wall decay equation:

$$\frac{dC_w}{dt} = -k_r C_w - d \cdot k_{mt}^e C_w \tag{3}$$

with C_w the chlorine concentration taking into account wall decay only (mg/L), k_r the stagnant decay rate (1/s), k_{mt} the coefficient of mass transfer to the pipe wall (m/s) and *d* and *e* parameters in the net wall decay function. For chlorine in PVC the wall decay can be assumed to be equal to zero, as was found by Clark et al. (2012; 2010). For unlined ductile iron pipes Clark et al. (2012) provided some values for reaction rate coefficients, which are primarily driven by corrosion. k_{mt} can be determined from the dimensionless Sherwood number *Sh*, the pipe diameter d_{pipe} (m) and diffusivity constant *D* (Table 1). *Sh* (Table 1) depends on the Reynolds number *Re* and the Schmidt number *Sc* (Table 1) which depends on the kinematic viscosity ν (Pa.s) and *D* (Rossman 2000). These equations show that the wall decay depends on the flow velocity.

The combined model of Vasconcelos et al. (1997) and Clark et al. (2012) is implemented in MSX as:

$$\begin{aligned}\frac{dC_{Cl}}{dt} &= -k_{20} \cdot \exp\left(\frac{-E/R \cdot (20 - T_{water})}{(273+20)\cdot(273+T_{water})}\right) C_{cl} + \\ &\quad -k_r C_{cl} - d \cdot k_{mt}^e C_{cl}\end{aligned} \tag{4}$$

Figure 1a) shows the results for chlorine decay for the different equations including the effect of bulk and wall decay and temperature dependence for PVC and CI pipes. Note that because C_w is neglected for PVC pipe (no wall reactions), there is no velocity dependence on the decay rate for PVC. Because the heat exchange is also driven by convection, there is a small influence from the temperature dependence of the velocity.

Blokker and Pieterse-Quirijns (2013) have described how to model the temperature of the water in the DWDS. The temperature model in MSX is defined as:

$$\frac{dT_{water}}{dt} = \frac{\alpha_{water}}{\left(d_{pipe}/2\right)^2 \left(\lambda^* + 1/Nu\right)} \left(T_{outer\ wall} - T_{water}\right) \tag{5}$$

with T_{water} the temperature of the drinking water in the DWDS (ºC), $T_{outer\ wall}$ the temperature of the soil surrounding the DWDS, α_{water} the thermal diffusion coefficient (m^2.s^{-1}) of water, *Nu* the Nusselt number (-). *Nu* depends on *Re* and therefore on the actual flow velocities. Furthermore, λ^* is the characteristic ratio (-) of thermal conductivity of water (λ_{water}, W.m^{-1}.K^{-1}) and pipe wall ($\lambda_{pipe\ wall}$, W.m^{-1}.K^{-1}) (Table 1).The ratio between pipe diameter (d_{pipe}, m) and thickness of the pipe wall ($d_{pipe\ wall}$, m) for water mains is typically in the order of 15 for Cast Iron Ø150 mm pipes to 38 for PVC pipes (http://www.gizmology.net/pipe.htm). For Cast Iron the convective term is dominant (Blokker and Pieterse-Quirijns 2013) and thus the exact value for $d_{pipe\ wall}$ is less important. Since $d_{pipe\ wall}$ is not available in EPANET, the typical ratio of 38 is used in MSX.

Table 1 summarises all the values that are used in the MSX model.

Table 1. List of symbols and their values.

	symbol	unit	description	value	reference
Temperature model	α_{water}	$m^2.s^{-1}$	thermal diffusion coefficient	$1.36\cdot 10^{-7}$	(Blokker and Pieterse-Quirijns 2013)
	λ_{water}	$W.m^{-1}.K^{-1}$	thermal conductivity of water	0.6	
	$\lambda_{\mathrm{pipe\ wall}}$	$W.m^{-1}.K^{-1}$	thermal conductivity of pipe wall	PVC 0.16 AC 0.43 lined Cast Iron 8.9	
	λ^*	-		$\dfrac{\lambda_{water}}{\lambda_{pipewall}} \dfrac{d_{pipewall}}{d_{water}}$	
	d_{pipe}	m	pipe diameter	from EPANET	-
	$d_{pipe\ wall}$	m	pipe wall thickness	d_{pipe} / 38	PVC PN10, ≥ Ø 90 mm Cast Iron: d_{pipe} / 15 for Ø150 mm, 300 kPa, http://www.gizmology.net/pipe.htm
	Nu	-	Nusselt number	$0.027 \cdot \mathrm{Re}^{0.8} \cdot \mathrm{Pr}^{0.33}$	-
	Pr	-	Prandtl number	7	$Pr \approx 7$ for T_{water} = 20 ºC
	Re	-	Reynolds number	from EPANET	-
	T_{water}	ºC	temperature of the drinking water in the DWDS	from EPANET MSX	Eq. (5)
	$T_{\mathrm{water,\ 0}}$	ºC	initial value of T_{water} at entry point	10	Assumed typical value
	$T_{\mathrm{outer\ wall}}$	ºC	temperature of the soil surrounding the DWDS	25	Assumed typical value
Chlorine model	C_{Cl}	$mg.L^{-1}$	concentration of free chlorine	from EPANET MSX	Eq. (4)
	$C_{Cl,\ PS}$	$mg.L^{-1}$	dose C_{Cl} at entry point	1.0	Assumed typical value
	$C_{Cl,\ min}$	$mg.L^{-1}$	minimum required C_{Cl} at customer	0.2	Assumed operational goal based on (USEPA 1989)
	D_T	$m^2.s^{-1}$	diffusivity constant of chlorine at temperature T	$\dfrac{T_{water}+20}{293} \cdot \dfrac{\nu_{20}}{\nu_T} \cdot D_{20}$	
	D_{20}	$m^2.s^{-1}$	diffusivity constant of chlorine at 20 ºC	$1.21\cdot 10^{-9}$	(Axworthy and Karney 1996)
	d	-	parameters in the net wall decay function, for chlorine in Cast Iron mains	0.032	(Clark et al. 2012), conversion because k_{mt} is in m/s (instead of cm/h) $0.17\dfrac{(3600 \cdot 100)^{0.51}}{3600}$
	e	-		0.51	(Clark et al. 2012)
	E/R	K	activation coefficient	12,104	doubling after 5 °C
	K_{T}	$L.mg^{-1}.s^{-1}$	reaction rate coefficient at temperature T	$k_{20} \cdot e^{\left(\frac{-E/R \cdot (20-T_{water})}{293 \cdot (273+T_{water})}\right)}$	(Vasconcelos et al. 1997)
	k_{20}	$L.mg^{-1}.s^{-1}$	base value at a reference temperature of 20 ºC	$1.0\cdot 10^{-5}$	0.87 per day, see text.
	k_r	s^{-1}	stagnant decay rate, for chlorine in Cast Iron mains	$2.0\cdot 10^{-5}$	0.074 per hour (Clark et al. 2012)
	k_{mt}	$m.s^{-1}$	coefficient of mass transfer to the pipe wall	$\dfrac{Sh \cdot D_T}{d_{pipe}}$	(Rossman 2000), Sh for Re > 2300
	ν_{T}	Pa.s	kinematic viscosity at temperature T	$\dfrac{497 \cdot 10^{-6}}{(42.5+T_{water})^{1.5}}$	
	Sc	-	Schmidt number	$Sc = \dfrac{\nu_T}{D_T}$	
	Sh	-	Sherwood number	$0.0149\,\mathrm{Re}^{0.88}\, Sc^{1/3}$	

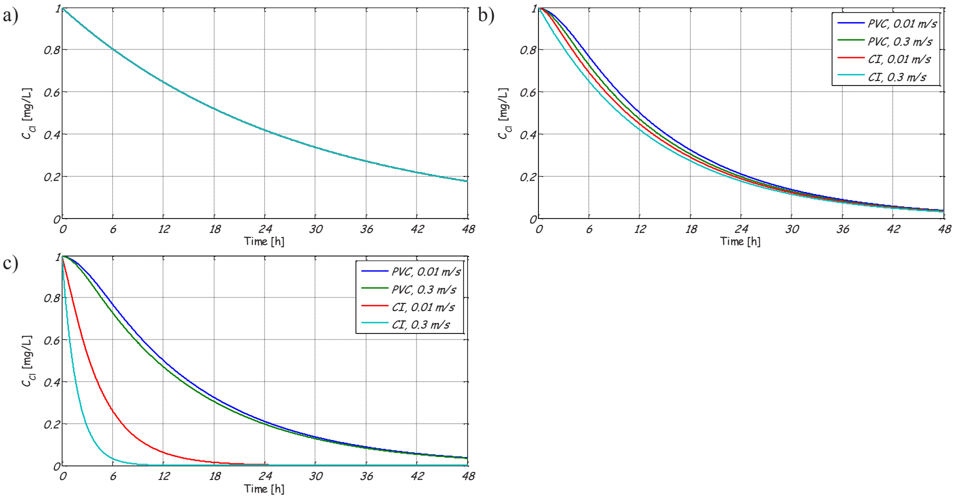

Figure 1. Chlorine decay over time for different pipe materials (PVC and CI) and flow velocities (0.01 and 0.3 m/s) with d_{pipe} = 152.4 mm for a) bulk decay only, Eq. (1); b) bulk decay with temperature dependence, Eq. (2) and (5); c) bulk and wall decay with temperature dependence, Eq. (4) and (5). Table 1 gives the values of the parameters.

2.2. Hydraulic network model

The selected case study network is situated in the Dutch town Zandvoort (Blokker et al. 2010a), along the sea. The network was built in the 1950-1960's and consists of 3.5 km of PVC pipes, and 5.7 km of lined cast iron pipes; it supplies about 1000 homes, 2 hotels and 30 beach clubs (Figure 2). The area is supplied from one point with a fixed head through a booster pump. The water use in the network is, on average, 24 m^3/h. Domestic water demand is 70% of the total demand. The drinking water is distributed without any disinfectant, as is common in the Netherlands, so model predictions were not able to be field verified for this study.

A previous study (Blokker et al. 2010a) describes the difference between the so-called top-down and bottom-up model. For this purpose, an "all pipes" hydraulic model of a DWDS was constructed with two types of demand allocations. One was constructed with the conventional top-down approach, i.e. a demand multiplier pattern from the booster station was allocated to all demand nodes with a correction factor to account for the average water demand on that node. The other was constructed with a bottom-up approach of demand allocation, i.e., each individual home was represented by one demand node with its own stochastic water demand pattern which were constructed with the drinking water demand model SIMDEUM (Blokker et al. 2010a; Blokker et al. 2010b). The bottom-up approach was tested with 10 different sets of randomly generated SIMDEUM demand patterns. In the autumn of 2008 a tracer test with sodium chloride was performed to measure travel times. It was concluded that the bottom-up model performs at least as well as the conventional top-down model with respect to total demand and travel times, without the need for any flow measurements or calibration measurements. The bottom-up model leads to a stochastic method of hydraulic modelling and gives insight into the variability of travel times as an added feature beyond the conventional way of modelling.

The same drinking water demand patterns in the top-down model (Model_{TD}) and bottom-up model (Model_{BU}, 10 runs) were used as in the reference paper, except that the constant demands of 0.04 m^3/h at the 4 measurement locations were excluded. And again, no leakage was assumed in this network. The demand pattern time step was set to 5 minutes as suggested by Blokker et al. (2011). The water quality time step was set to 1 minute. Typical travel times are 2 to 45 hours on the measurement locations in a previous study (Blokker et al. 2010a).

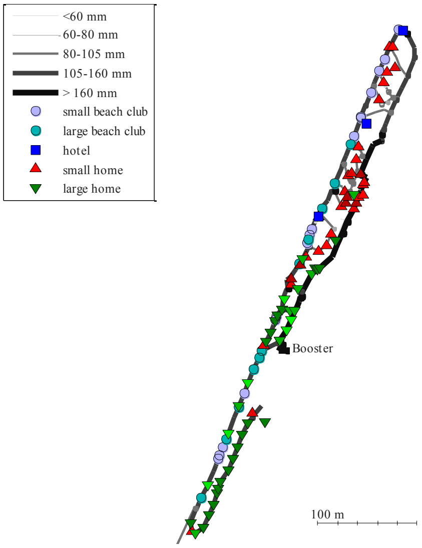

Figure 2. Zandvoort Network. The line thickness indicates the pipe diameters. The symbols indicate the different types of customers. The brightness of the colours of the homes indicates the number of household connections per node; bright red e.g. indicates an apartment building.

2.3. Evaluation parameters

A typical operational goal for water utilities is to maintain a minimum chlorine residual of 0.2 mg/L (USEPA 1989) so that value was selected as a threshold for this study. The number of non-zero demand nodes that do not comply with this level, even for only for part of the day, are counted. The demand nodes are weighted by number of customer connections: each residential connection is counted as 1, hotels and beach clubs are taken as equivalent households based on their daily water use (a household has a daily water use of ca. 370 L).

Table 2 summarizes the simulations performed with different chlorine decay model components.

Table 2. Summary of model simulations performed

MSX scenario	**Chlorine model**	**Temperature dependence**	**hydraulic model**
1_TD	Bulk decay only, Eq. (1)	Constant temperature, T_{water} = 20 °C	$\mathrm{model}_{\mathrm{TD}}$
1_BU			$\mathrm{model}_{\mathrm{BU}}$
2_TD	Bulk decay only, Eq. (2)	Variable temperature, Eq. (5)	$\mathrm{model}_{\mathrm{TD}}$
2_BU			$\mathrm{model}_{\mathrm{BU}}$
3_TD	Bulk decay and Wall decay, Eq. (4)	Variable temperature, Eq. (5)	$\mathrm{model}_{\mathrm{TD}}$
3_BU			$\mathrm{model}_{\mathrm{BU}}$

TD = top-down demand model, BU = bottom-up demand model

3. Results and discussion

The model simulation produces a predicted residual chlorine concentration at each node. Figure 3a)-d) shows the results of the bulk decay model at 20 ºC at 4 locations for the $\mathrm{Model}_{\mathrm{TD}}$ and 10 different runs of $\mathrm{Model}_{\mathrm{BU}}$. In general, the two demand models produce similar trends when only bulk decay at a fixed temperature is considered. However, at location 4 the minimum chlorine concentration of 0.2 mg/L is not always maintained, depending on the individual household water use as shown in different $\mathrm{Model}_{\mathrm{BU}}$ simulations. Figure 3e) zooms in on this location. For 7 of the 10 $\mathrm{Model}_{\mathrm{BU}}$ simulations, the minimum chlorine level is maintained but for the other 3 runs, there is a part of the day where this is not the case: the target concentration is not reached during 0.7%, 1.0% or

56% of the day. Depending on the criterion for maintenance of chlorine residual, this particular node could be considered to have violated operational goals. For the case study system, location 4 is an apartment building with 15 homes, which represents 1% of the total customer connections.

The result of the Model$_{BU}$ runs can then be converted into a box and whisker plot (Figure 4) that presents the results for all demand nodes, while taking into account the criterion for how often the threshold value may be exceeded.

- If the criterion for reaching the threshold is set at 0, i.e. the threshold should be exceeded at all times during the day, then node 4 would contribute with 1% of all customer connections to the positives for 3 out of 10 runs. Figure 4 shows that for 0 % allowed exceedance for each of the 10 model$_{BU}$ runs at least 0.4 % of all customer connections do not comply and in some runs 1.6% do not comply (1% from node 4).
- If the criterion for reaching the threshold is set at 0.1, this means that the threshold should be exceeded at 90% of the day, then node 4 would contribute with 1% of all customer connections to the positives for 1 out of 10 runs. Figure 4 shows that for 10 % allowed exceedance for each of the 10 model$_{BU}$ runs at least 0.4 % of all customer connections do not comply and in only one run 1.6% do not comply (1% from node 4).
- If the criterion for reaching the threshold is set at 0.2 to 0.5, then node 4 would contribute with 1% of all customer connections to the positives for 1 out of 10 runs. Figure 4 shows that for 50% allowed exceedance for each of the 10 model$_{BU}$ runs at least 0.2 % of all customer connections do not comply and in only one run 1.4% do not comply (1% from node 4).
- If the criterion for reaching the threshold is set at 0.6 or more, then node 4 would not contribute to the positives for any of the 10 runs (not shown in Figure 4).

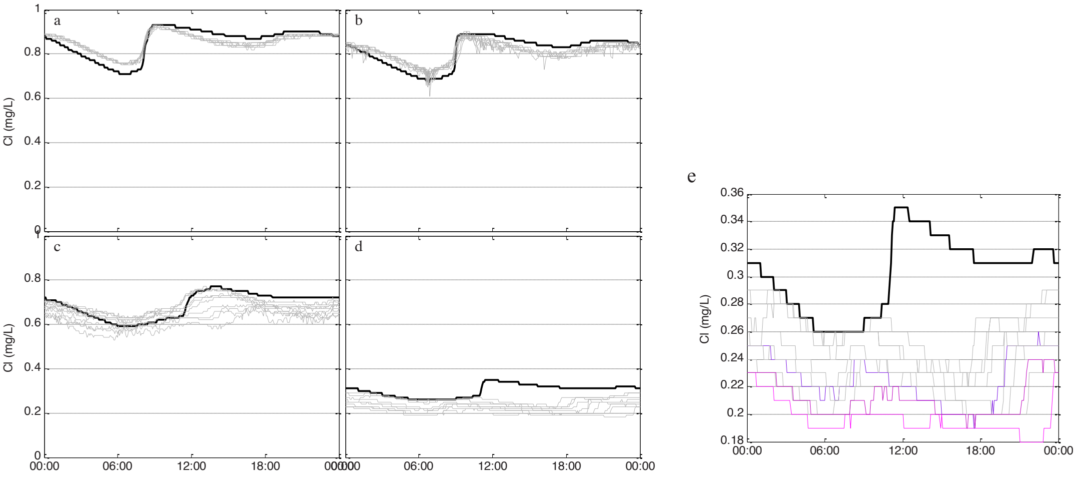

Figure 3. Modelled residual chlorine with the chlorine bulk decay model at 20 ºC at locations a) 1, b) 2, c) 3, d) 4 (Blokker et al. 2010a) and e) 4, zoomed in from d. The black line is the result of the Model$_{TD}$ run, the gray lines are the results of the 10 different Model$_{BU}$ runs. The three purple lines in e) show that at some point during the day, the minimum chlorine level of 0.2 mg/L is not maintained.

The results from the Model$_{BU}$ runs shown in Figure 4 also illustrate both the predicted chlorine concentrations and the duration of the threshold violation when chlorine falls below the target of 0.2 mg/L. These figures alsoshow the fraction of customers where chlorine concentration is lower than the threshold concentration for different time durations. For example in Figure 4a) for bulk decay at a fixed temperature (scenario 1), the minimum chlorine concentration threshold was not maintained for a duration 10% of a day (144 minutes) at approximately 0.4% of customer locations (fraction = 0.004) in the Model$_{TD}$. The Model$_{BU}$ produced a similar median result for the duration of 10% of a day in this case with bulk decay only. The results for zero duration show that 0.4% of customers did not meet the minimum concentration threshold at any time during the day based on the Model$_{TD}$, compared to 0.6% of customers with the Model$_{BU}$.

Figure 4b) and c) provide box and whiskers plots for scenarios 2 and 3, which include temperature variation and wall decay in addition to bulk chlorine decay. In these scenarios, the water temperature at the point of entry to the system is 10 °C and increases according to Eq. (5) to a maximum of 25 °C as dictated by the assumed soil temperature. The results for scenario 2 in Figure 4b) demonstrate that including the temperature variation in the distribution system has a significant impact on results for both the Model_{TD} and Model_{BU}. To compare with Figure 4a) for zero duration, the Model_{TD} predicts that 33% of customers would not meet the 0.2 mg/L threshold at any time versus 0.4% when temperature is fixed at 20 °C. The Model_{BU} for zero duration predicts that slightly fewer customers, only 30%, would not meet the threshold. In general, the Model_{BU} results in a lower temperature increase and therefore a slightly less aggressive chlorine decay than the Model_{TD}.

Figure 4c) illustrates the significance of the wall decay. In Figures 4a) and b), the results are fairly similar for all time durations, indicating that a certain number of customer locations are receiving low chlorine water for a longer period of time. In Figure 4c), the inclusion of wall decay has resulted in a larger number of customers (42% for the Model_{TD}) receiving low chlorine concentrations for the full day but fewer customers receiving low chlorine water for partial days (only 0.5% not meeting threshold for half of the day). The Model_{BU} results in fewer customers (median of 25%) with low chlorine for the full day but the results for the two demand models are similar as the threshold duration increases, i.e. for those locations that have low chlorine concentrations for partial days.

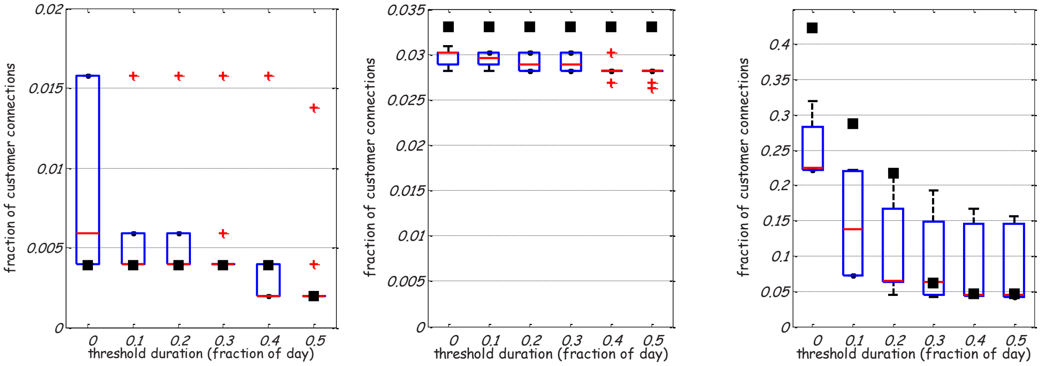

Figure 4. Fraction of customer connections not maintaining the threshold of 0.2 mg/L during a given fraction of the day as a result of a) the chlorine bulk decay model at 20 ºC (scenario 1); b) the chlorine bulk decay model at variable temperature (scenario 2); c) the chlorine bulk and wall decay model at variable temperature (scenario 3). The black squares are the results from the Model_{TD}; the box and whisker plots are the results from the 10 Model_{BU} runs. The boxes represent the 25th-75th percentile; horizontal lines within the boxes represent medians; whiskers extend 1.5 times the length of the interquartile range above and below the 25th and 75th percentiles; and outliers are represented as plusses.

The box and whisker plots of Figure 4 show how the variability of demand results in the variability of residual chlorine. The effect is the largest in the case where wall decay plays a role. When chlorine measurements in the DWDS are used for model calibration purposes, it should be noted that the uncertainty in both the decay model and in demand are important factors to take into account. Pasha and Lansey (2010) also have shown that water quality predictions of residual chlorine in a DWDS are very sensitive to uncertainty in demand and the bulk and wall reaction coefficients, and not very sensitive to pipe diameter and wall roughness. Calibration of the diameter and wall roughness by means of pressure measurements may therefore not be required. Jonkergouw et al. (2008) showed that calibration of demands can be done by using water quality measurements (in their case chlorine levels). They concluded that average daily demands can be determined with high precision, but that substantial measurement errors in the calibration data (i.e. water quality data) do not allow for an accurate calibration of the demand multiplier patterns (hourly). Our results suggest that the stochastic nature of demand may also impede accurate calibration, because the demand multiplier pattern is highly variable and therefore the residual chlorine levels are as well, particularly when wall decay reactions are considered. Water quality measurements are preferably used for the calibration of reaction coefficients but not also for the calibration of demands.

4. Conclusions

This study examined the impact of stochastic demand modelling on chlorine predictions using several different chlorine decay model formulations. The results presented here are specific to the case-study system but give an illustration of how the inclusion of stochastic demand and temperature effects might influence chlorine predictions. In particular, temperature is often overlooked but can have a significant impact. One important finding is that the selection of the chlorine decay model formulation has a greater impact on the results than the demand model. The demand model has a small effect in combination with the bulk decay model at constant temperature: the traditional (top-down) approach of modelling can result in a higher chlorine concentration (Figure 3e), but not at all locations within the DWDS and not consistently throughout the day (Figure 3a-d). Including the wall decay has a significant impact on predicted chlorine concentrations but only at certain locations in the DWDS. The stochastic (bottom-up) approach of modelling can help clarify the residence time, and therefore the duration of low chlorine concentration events, which is important at the worst locations (Figure 4c). The inclusion of stochastic demand models in conjunction with increased and site-specific knowledge about chlorine reactions will be necessary to achieve a new level of confidence in water quality model predictions.

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