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Impact of pipe material on the wall reaction coefficients and its application in the rehabilitation of water supply system of San Pedro Nexapa, State of Mexico

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ABSTRACT

One of the major challenges faced by water companies around the world is the high level of chlorine losses in distribution networks. This paper presents an experimental study to examine chlorine loss in different types of pipe materials and select the ones with low chlorine demand for the rehabilitation of the water distribution network of San Pedro Nexapa, State of Mexico. The materials investigated include: polyvinyl chloride (PVC), galvanized steel (GS), polypropylene (PP) and high-density polyethylene (HDPE). A 24-h chlorine consumption study was performed in a simulated water distribution network to assess the impact of wall reaction coefficient on chlorine decay. Four sets of independent pipe loops of 50 mm in diameter and 12 m in length were used. Two different scenarios were considered based on different initial chlorine concentration (1.21 mg/L and 1.60 mg/L). Samples were collected at each loop at two-hour intervals and physicochemical analyses were conducted. Results from the experimental distribution network showed that the wall coefficient values for GS, HDPE, PP and PVC were 0.165 h^{-1}, 0.059 h^{-1}, 0.043 h^{-1} and 0.026 h^{-1}, respectively. Experimental results showed that wall reaction coefficient values depend on initial chlorine concentration and the characteristics of pipe material. The rate of free chlorine decay was found to be faster in steel pipe and slower in the plastic pipes. Based on its having the lowest chlorine demand compared with the other pipes, PVC pipe would be selected to rehabilitate Nexapa water distribution network, State of Mexico. The wall coefficients from the experimental study were incorporated into EPANET through four simulation runs to predict chorine decay of San Pedro Nexapa water distribution network, State of Mexico. In the PVC and PP pipes higher residual chlorine concentrations were observed that ranged from 0.30 to 0.90 mg/L and 0.50 to 0.95 mg/L, respectively. This study is important for utilities to operate their system effectively and protect public health.

Key words: chlorine decay, EPANET, pipe material, rapid reactions, slow reactions, wall reactions

HIGHLIGHT

- Results of this study are useful to understand the effect of wall reaction coefficient (k_w) values on chlorine decay and could help develop better management systems to address issues associated with chlorine decay in water distribution systems.

INTRODUCTION

Chlorine is a strong oxidant commonly used in water during the disinfection process (Fisher *et al.* 2017). It is used to control biofilm growth and to inhibit microbial activity in the network system. While flowing through pipes, however, the chlorine concentration decreases owing to its strong oxidant properties and decay behaviour in the bulk solution and wall interaction. Water distribution systems are designed to meet safe drinking water quality standards and should be capable of meeting the demand at all times with satisfactory pressure. However, the management of water distribution infrastructure to ensure customer satisfaction is becoming very complex. Population growth and expansion of urban development in large cities require

expansion of existing water distribution systems to meet the increased demand while maintaining the desired water quality in spite of aging infrastructure. In this case, it is always proposed to add new pipe segments.

To simulate water quality in a network, most software packages such as EPANET model the decay of chlorine using a bulk decay rate and a wall decay coefficient (Rossman *et al.* 1994; Ramos *et al.* 2010; Fisher *et al.* 2017). Bulk decay accounts for the loss of chlorine corresponding to the aging water within the distribution system; wall decay is the loss of chlorine due to the interaction of the flowing water with the pipe wall. Typically, the bulk decay rate is calculated based on bottle tests for each source of water. In the case of a single water source, the decay rate is uniformly assigned to the entire distribution system. If there are multiple sources, the decay rate is assigned to the areas served by each source.

Bulk decay depends on the amount and type of natural organic matter and inorganics in water; hence, water samples should be collected and laboratory decay tests carried out for assessing decay kinetics, by means of the bottle tests (Powell *et al.* 2000).

Many studies were conducted to determine the bulk chlorine decay (Hallam *et al.* 2002; Neupauer 2010; Ammar *et al.* 2014). Wall decay, however, depends on the pipe material and its conditions (Nejjaria *et al.* 2014). The determination of the wall coefficient is often obtained either by performing laboratory study, by using a pipe loop system constructed with 30-year-old pipes (or older), or through field study (Karadirek *et al.* 2016). Because of the complexity of the water distribution systems, however, only a few studies have been performed. The objective of this study is to estimate wall reaction cofficients of different pipe materials in an experimental setup and to use the values in EPANET simulation of a real water distribution network in San Pedro Nexapa, State of Mexico.

Currently, for the expansion or rehabilitation of an existing network, water supply authorities in Mexico use high-density polyethylene (HDPE), polypropylene (PP) and polyvinyl chloride (PVC) pipes because of their flexibility during earthquake events, their strength and their durability. Their performance in terms of maintaining residual chlorine in the network needs to be carefully examined. Based on laboratory experiments and EPANET model simulation, this study will be useful to select the best pipe material based on low chlorine demand for the rehabilitation of the water distribution network of San Pedro Nexapa, State of Mexico.

MATERIALS AND METHODS

Experimental setup and preparation

To estimate the wall reaction coefficient, a series of experiments were carried out using an experimental setup, which consisted of three parts (see Figure 1):

(1) A water reservoir of 2.12 m^3 of capacity, (2) a storage tank (450 L capacity) at elevated position for gravity flow and (3) a pipe network consisting of four sets of independent loops of 50 mm diameter and 12 m length of PVC galvanized steel (GS), PP and HDPE.

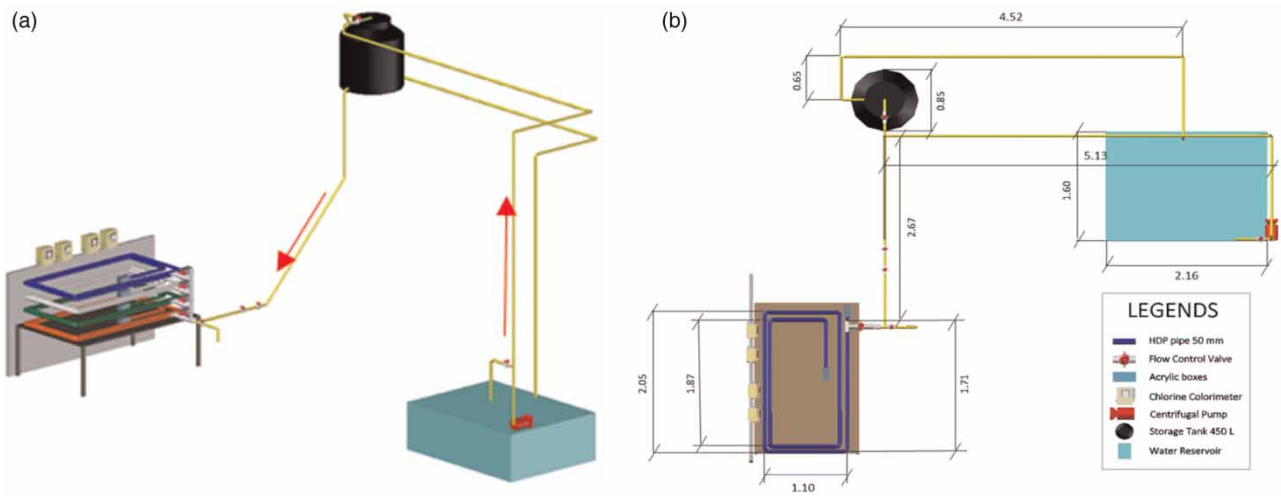

Figure 1 | Schematic diagram of the laboratory scale water distribution network: (a) side view (3D) and (b) top view (2D).

The network included nine flow control valves to fill and drain the system and an online CL763 (B&C Electronics, Italy) chlorine analyzer installed in each loop, which can detect chlorine concentration in the range from 0.1 to 20 mg/L. Four data logger (El-USB-4, Lascar Electronics, USA) connected in each chlorine analyzer recorded data over time; a manual mixer was installed at the storage tank to get a homogeneous mixture of tap water and chlorine. A 4HME200 centrifugal pump was used to transfer water from the reservoir to the elevated storage tank.

Each loop was first flushed with clean water (free of chlorine) for approximately 10 minutes. Then the loop was filled with water from the storage tank. At the extreme ends of each loop were located two 0.18 m × 0.09 m acrylic boxes. Each box was equipped with a mini (4–203, Aquakril) submersible water pump, which takes samples to the chlorine analyzer (overflow cell) through a 1/4' connection tube. The cell's manufacturing characteristics allow the sample to run through the (sensor) potentiostatic electrode site with a constant velocity then exit through a 10 × 14 mm tubing to the second acrylic box (located on the other extreme end of the loop).

Experimental procedure

Experiments were performed in an attempt to estimate the wall reaction coefficient in four different new pipe materials as a function of initial chlorine concentration. Non-chlorinated water was pumped from the 2.13 m^3 reservoir to the elevated storage tank by using the 4HME200 centrifugal pump. Samples were chlorinated with 13% free chlorine (sodium hypochlorite) solution. K-Tonic solution, which is a mix of six compounds of total nitrogen, urea nitrogen, K_2O, extract of total humic carbon, humic acid carbon and fulvic acid carbon, was used as contaminant agent (1.50 mg/L in each scenario). Two scenarios were run at an initial chlorine concentration of 1.21 (scenario 1) and 1.60 mg/L (scenario 2), since in the case of water supply in certain places in the world, the water leaving the treatment plant typically has an initial chlorine concentration in these concentration ranges.

To get a homogeneous mixture of tap water and chlorine, a manual mixer was used at the storage tank. Water was continuously recirculated in the simulated distributions system. The chlorine decay was determined continuously as samples ran through the sensor. Upon activation, data loggers were deployed to measure and record chlorine concentration at two-hour intervals for the duration of the monitoring period, which lasted for 24 hours. Once the experiments were completed, a software was used to download and analyze the collected data. To ensure that the results are reliable, each experiment was conducted in triplicate.

Analytical method

Chlorine decay kinetics

Because chlorine can be transported from the bulk flow to the pipe wall, the overall rate coefficient can be defined as a combination of the effects of bulk reaction, wall reaction and mass transfer (Rossman *et al.* 1994) and can be expressed as:

$$\frac{dC}{dt} = -\left(k_b + \frac{k_w k_f}{r_h(k_w + k_f)}\right)C \tag{1}$$

where k_b: bulk decay rate constant; k_w: wall decay constant; k_f: mass transfer coefficient; r_h: hydraulic radius of the pipe and C: chlorine concentration.

Standard literature expressions can be used for the mass-transfer coefficient k_f (Edwards *et al.* 1976):

$$k_f = Sh\frac{D}{d} \tag{2}$$

where d: diameter of the pipe and D: the molecular diffusivity and it is the Sherwood number, which could be expressed as:

$$Sh = 0.023\mathrm{Re}^{0.83}Sc^{0.33}; \quad \text{for Re} > 2300 \tag{3}$$

in which Re is the Reynolds number and Sc is the Schmidt number. For Re <2300, the Sherwood number can be expressed as follows:

$$Sh = 3.65 + \frac{0.0668(d/L)\mathrm{Re}Sc}{1 + 0.04[(d/L)\mathrm{Re}Sc)]^{2/3}} \tag{4}$$

in which L is the length of the pipe.

With the first-order wall reaction, the rate expression (Equation (1)) can be simplified

$$\frac{dC}{dt} = -KC^n \tag{5}$$

After separating variables and integrating, Equation (5) becomes

$$C = C_0 \exp - (kw)t \tag{6}$$

in which C: final chlorine concentration (mg/L); C_0: initial chlorine concentration (mg/L); k_w: wall reaction coefficient (h^{-1}) and t: time (h).

Water quality analysis

Temperature and pH were measured using a 350 mercury thermometer (Lauka, USA) and a M530P (Pinnacle Series, USA) unit. The average temperature of the water for all the tests varied within the range of 15–20 °C. Turbidity was measured using a turbidimeter (2100A, HACH, Mexico).

RESULTS AND DISCUSSIONS

Scenario 1

Under this scenario, experiments were carried out in triplicate where water samples were dosed with initial chlorine concentration of 1.21 mg/L. The mean chlorine concentration was calculated on the basis of the set of data of each material to examine the wall reaction coefficient. Other parameters such as turbidity, pH and temperature were taken into consideration. Mean values of triplicate samples were used in plotting chlorine concentration as a function of time. An exponential adjustment was made to obatin the wall reaction coefficient for each sample. The experimental results for scenario 1 revealed the effect of pipe material on the rate of decay. Complete chlorine decay was observed in 24 hours in the GS pipe loop. In the other pipe loops only slight changes were observed from 8 to 24 hours. Figure 2 shows chlorine decay observed and curve

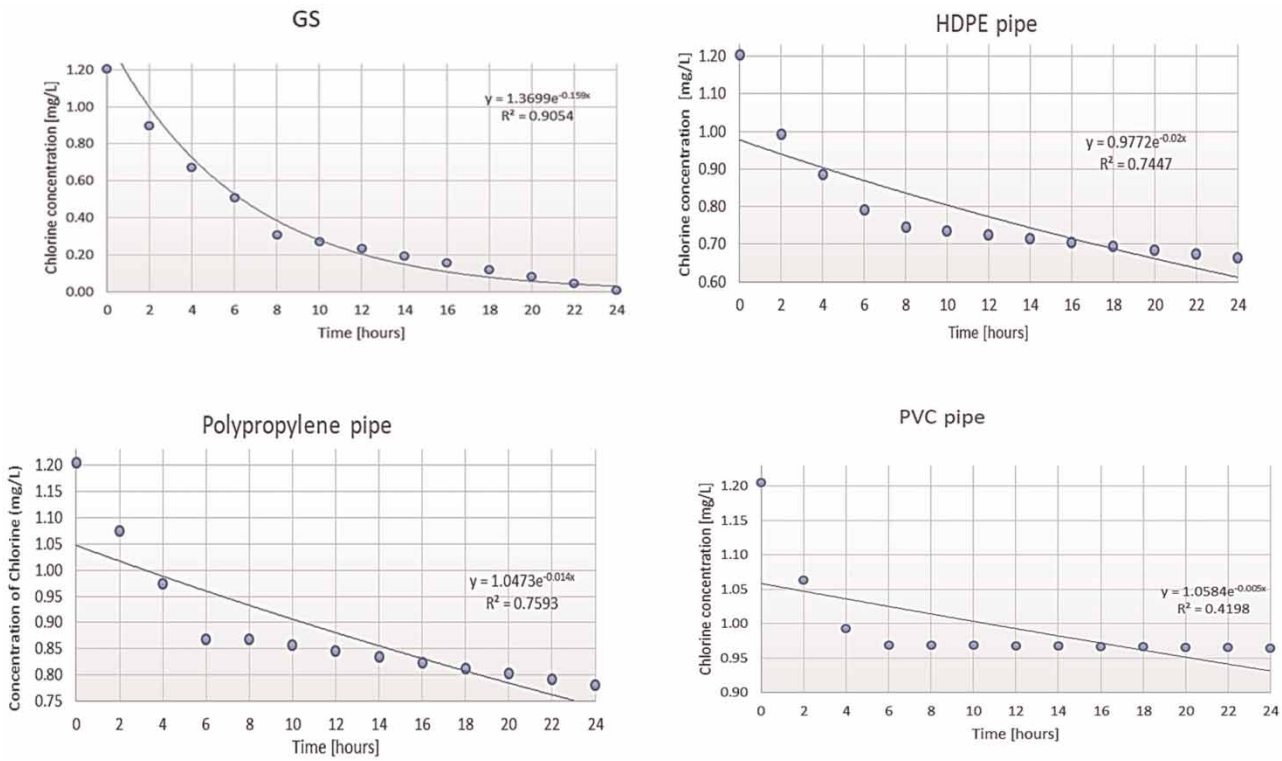

Figure 2 | Chlorine decay observed and curve fitting in samples collected in the pipe loop (24 h).

fitting in samples collected in the pipe loop (24 h). It was observed that chlorine reacted differently in the four pipe materials. The ranking of chlorine decay rate in the pipe loop system was as follows: GS pipe > HDPE pipe > PP pipe > PVC pipe, and might be caused by the reaction of chlorine with the material itself and the temperature since parameters such as pH and turbidity remained constant during the experiments. A similar trend was observed by Aravelo (2007) where results of his study showed that the rate of chlorine decay was found to be highly affected by the pipe material and the decay was faster in steel pipe and slower in the synthetic pipes. Saeed *et al.* (2015) carried out laboratory experiments to measure the changes in concentrations of residual chlorine with time under a variety of conditions. The study indicated that the prominent factors that affect chlorine decay included initial chlorine dosage, temperature, pH and the amount of natural organic matter (NOM).

As shown in Figure 2, the trend lines did not fit the data perfectly. Poor R-square values were observed in the PVC, HDPE and PP pipes, respectively. This could be explained by the fact that chlorine decays more rapidly during the first eight hours and very slowly for the remaining time. Since the initial chlorine decay is 'fast' at the beginning and 'slow' at the end, it was suggested to divide the series of chlorine concentration data into two phases: the fast phase where the fast consumption was observed and, the slow phase where a gradual consumption was observed (Saeed *et al.* 2015). In this study, for each experiment, the data series were divided into two phases, then the wall reaction coefficient k_f for the fast phase (0–8 h) and k_s for the slow phase (8–24 h) were estimated. Figure 3 shows the free chlorine decay profile of water in the fast phase only. The profiles for the slow phase followed similar pattern as in the fast phase. The values of the wall decay constant as well as R-squared obtained in each pipe loop are summarized in Table 1.

The ranking of the wall reaction coefficient (k_w) in the pipe loop system for the whole phase (24 h) as well as the fast phase (8 h) was as follows: GS > HDPE > PP > PVC. A similar trend was observed in the slow phase (8–24 h) as well. A combination of first- and second-order kinetic models was used to predict chlorine concentrations. The first-order kinetic model was used to predict the fast phase as shown in Equation (7).

$$C = C_0 \exp(-k_f t) \tag{7}$$

in which k_f is the wall reaction coefficient for the fast phase. For the slow phase, the second-order kinetic model was used to predict the residual chlorine concentration. According to Powell *et al.* (2000), second-order equation can be

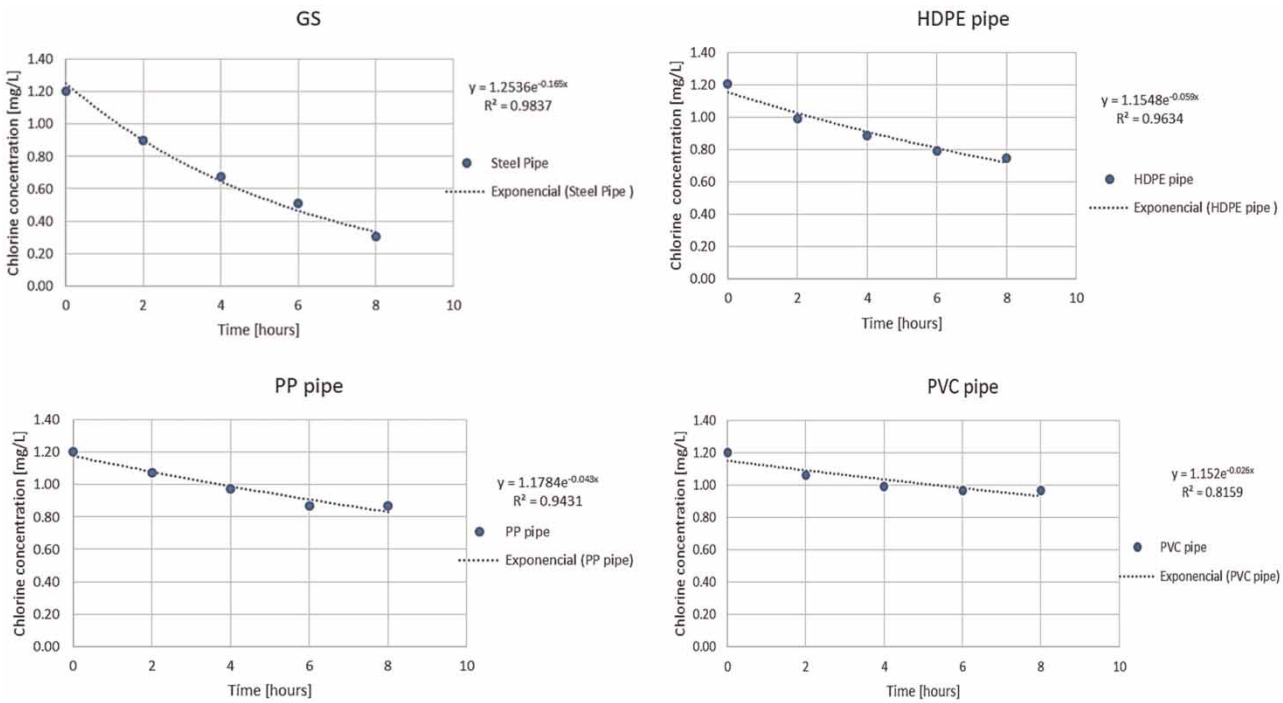

Figure 3 | Chlorine decay observed and curve fitting in sample collected in steel, PVC, PP and HDPE pipe (fast phase 0–8 h).

Table 1 | The values of the wall decay constant as well as R-squared obtained in each pipe loop for two reaction times: (a) 0–24 hours; (b) 0–8 hours

	A. Reaction time: 0–24 hours		B. Reaction time [0–8 hrs]			
Pipe material	**K_w [h^{-1}]**	**R^2**	**k_f [h^{-1}]**	**R^2**	**k_s [h^{-1}]**	**R^2**
GS pipe	0.043	0.82	0.165	0.98	0.007	1
HDPE	0.020	0.74	0.059	0.96	0.004	1
PP pipe	0.015	0.76	0.043	0.94	0.002	1
PVC pipe	0.006	0.42	0.026	0.82	0.001	1

expressed as:

$$C = \frac{C_0}{1 + C_0 k_s t} \tag{8}$$

Table 2 shows the results obtained using the combined first- and second-order chlorine decay model. Predicted chlorine residual concentrations were then compared with measured chlorine residual concentrations.

Base on the two phase approach (fast and slow phases) a good fit was observed between predicted and measured data. Absolute errors between 0 and 0.09 were observed with the combination of first- and second-order kinetic models as shown in Table 2.

Scenarios 2

In this scenario an initial chlorine concentration of 1.60 mg/L was used. Like in scenario 1, an exponential adjustment was made to obtain the reaction coefficient k_w for each sample. Figure 4 shows chlorine decay observed and curve fitting in samples collected in GS, HDPE, PP and PVC pipes for the fast phase (0–8 h).

In the equations presented in Figure 4, it is observed that the wall decay coefficient associated with the four pipe materials (k_w) ranged from 0.032 to 0.121 h^{-1} in the fast phase and from 0.001 to 0.007 h^{-1} in the slow phase. The results for the two phases are presented in Table 3.

In both scenarios, the GS pipe had a higher wall reaction coefficient, which resulted in a greater level of chlorine decay in the GS pipe, which resulted in a higher wall reaction coefficient. It is important to note that initial chlorine concentration has an impact on k_w values. Results of both scenarios are in agreement with the findings of Kiene *et al.* (1993), who demonstrated

Table 2 | Comparison between measured and estimated data using k_f and k_S

Slow phase (first order kinetic model)				**Cl_2 measured [mg/L]**					**Cl_2 predicted [mg/L]**							
HDPE	**GS**	**PP**	**PVC**	**Time**	**HDPE**	**Steel**	**PP**	**PVC**	**HDPE**	**GS**	**PP**	**PVC**	**Absolute error**			
0.059	0.165	0.043	0.026	0.00	1.21	1.21	1.21	1.21	1.21	1.21	1.21	1.21	0.00	0.00	0.00	0.00
0.059	0.165	0.043	0.026	2.00	0.99	0.90	1.08	1.06	1.08	0.87	1.11	1.14	0.09	0.03	0.03	0.08
0.059	0.165	0.043	0.026	4.00	0.89	0.67	0.97	0.99	0.96	0.63	1.01	1.09	0.07	0.05	0.04	0.09
0.059	0.165	0.043	0.026	6.00	0.79	0.51	0.87	0.97	0.85	0.45	0.93	1.03	0.06	0.06	0.06	0.06
0.059	0.165	0.043	0.026	8.00	0.74	0.31	0.87	0.97	0.75	0.32	0.85	0.98	0.01	0.02	0.01	0.01
Fast phase (second-order kinetic model)				**Cl_2 measured [mg/L]**					**Cl_2 predicted [mg/L]**							
HDPE	**GS**	**PP**	**PVC**	**Time**	**HDPE**	**Steel**	**PP**	**PVC**	**HDPE**	**GS**	**PP**	**PVC**	**Absolute error**			
0.004	0.007	0.002	0.001	10.00	0.73	0.27	0.86	0.97	0.71	0.26	0.86	0.97	0.02	0.01	0.00	0.00
0.004	0.007	0.002	0.001	16.00	0.7	0.16	0.82	0.97	0.67	0.16	0.82	0.97	0.03	0.00	0.00	0.00
0.004	0.007	0.002	0.001	24.00	0.66	0.01	0.78	0.97	0.62	0.01	0.78	0.97	0.04	0.00	0.00	0.00

HDPE, GS, PP and PVC pipe loop Cl_2 initial = 1.21 mg/L.

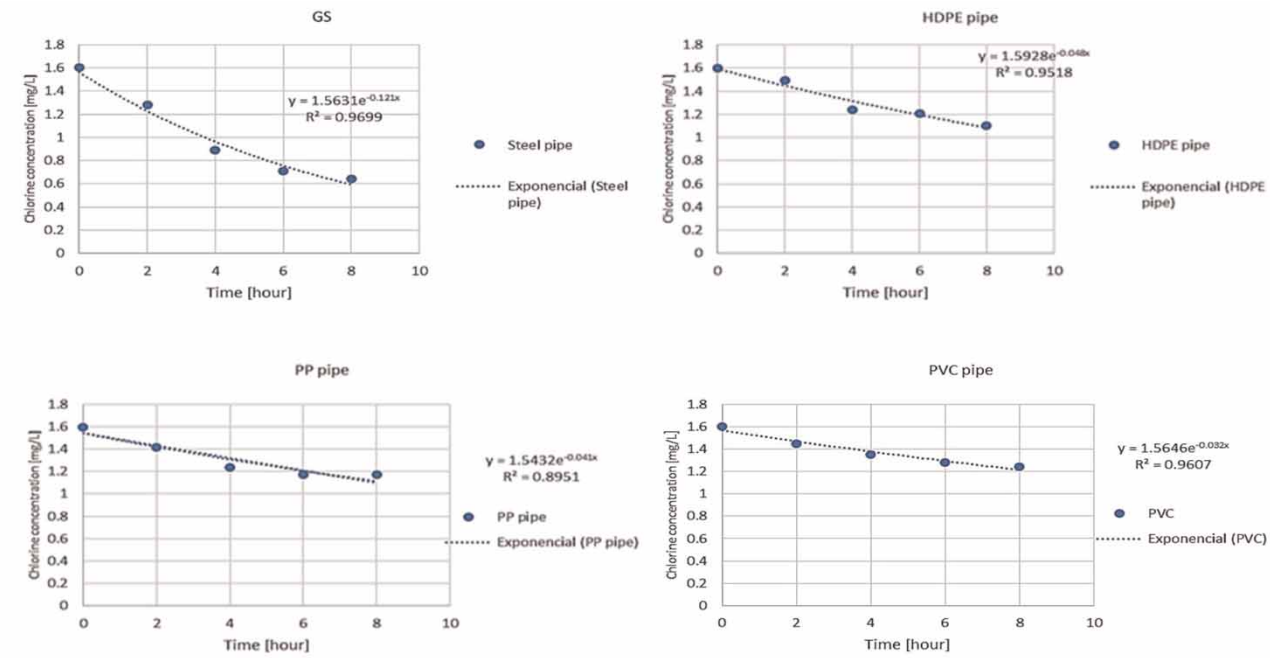

Figure 4 | Chlorine decay observed and curve fitting in simple collected in the pipe loop (fast phase 0–8 h).

Table 3 | Wall reaction coefficient for the fast and slow phases in scenario 2

Pipe material	k_f (0–8 h) [h^{-1}]	R^2	k_s (8–24 h) [h^{-1}]	R^2
GS pipe	0.121	0.96	0.007	1
HDPE Pipe	0.048	0.98	0.007	1
PP pipe	0.041	0.95	0.005	1
PVC Pipe	0.032	0.97	0.001	1

that the wall reaction rate constant for chlorine increases with decreasing initial chlorine concentration, (GS and HDPE in this study). The usual explanation for this is that chlorine decay rate may be influenced by chlorine concentration and NOM. A similar conclusion was also reached by Tonev & Dimova (2020), who investigated the chlorine wall decay in an old decommissioned metallic pipe using a pipe section reactor. A series of experiments were performed with different initial chlorine concentrations in the range 0.30 to 1.80 mg/L. The values of the wall reaction coefficient varied between 0.008 and 0.030 h^{-1}, decreasing exponentially with increasing initial chlorine concentration.

The wall reaction coefficient value for GS pipe was equal to 0.043 h^{-1} during the 24-h chlorine consumption study. This result agrees with that obtained by Monteiro *et al.* (2014), a k_w value of 0.040 h^{-1}. However, by taking into account the two-phase approach (fast and slow phases), k_w values increase during the 8 h chlorine consumption (0.121 and 0.165 h^{-1}). Wall reaction coefficient values for HDPE pipe obtained in this study varied between 0.041 and 0.059 h^{-1}. These values are greater than the calibrated wall decay coefficient estimated by Minaee *et al.* (2019) in a real-life drinking water distribution network, which ranged from 0 to 0.021 h^{-1}. Comparing the results of both studies, it would be understood that k_w reduces as diameter increases. On the other hand, the wall decay coefficients are considerably affected by the age, initial chlorine concentration, material type, diameter, roughness (Al-Jasser 2007), water temperature and the chemical and physico-chemical parameters of water (Digiano & Zhang 2005; Rossman 2006).

Finally, the k_w values for PVC pipes varied between 0.028 and 0.032 h^{-1} and are greater than the values obtained by Garcia Ávila *et al.* (2021), which ranged from 0.0001 to 0.0046 m h^{-1} and may be attributed to the length and diameter of the pipe material. In their study, pipe material range from 32 to 315 mm in diameter and 416 to 3,050 m in length.

APPLICATION IN A REAL WATER DISTRIBUTION NETWORK

To see the impact of wall coefficient associated with different pipe materials on chlorine decay, results obtained experimentally were used to simulate chlorine decay of San Pedro Nexapa water distribution network, State of Mexico using EPANET model.

San Pedro Nexapa is a small city located in the Municipality of Amecameca in the State of Mexico, with approximately 5,441 people in 2020. The water distribution network is supplied by an elevated reservoir, situated at 2,723 m above sea level, which is connected to a water treatment plant and supplies water to consumers by gravity. Average chlorine concentration at the outlet of the reservoir was 1.50 mg/L. The network also included a flow control valve along with 75 nodes and 122 pipes with a diameter ranging from 150 to 300 mm. Water demand was associated with each node of the model according to the population, depending on land use. Numerical simulations were performed using four different wall reaction coefficients that were obtained from the experimental study described earlier. The EPANET model representing the layout of the distribution network for the case study is shown in Figure 5.

To evaluate the variation of chlorine loss within the distribution system, four sampling sites (junctions) labeled N81, N21 N68 and N40, located respectively at the north, east, west and centre of the network were selected. Numerical simulations were carried out, wall reaction coefficients associated with the pipe material in the experimental study and a global bulk coefficient (0.033 h^{-1}) were incorporated in EPANET to evaluate chorine decay. Numerical simulations were conducted over a period of 24 hours. The variation of chlorine concentrations at each junction for the different simulations are presented in Figure 6. Water age at the sampling points (N68, N40, N21 and N81) are 10, 11, 14.50 and 24 hours, respectively.

Figure 6 shows that first simulation run was associated with the higher wall decay constant (0.165 h^{1}). In this case, chlorine concentrations ranged from 0.15 to 0.75 mg/L and were shown to be lower at site N81 (0.15 mg/L), followed by N21 (0.61 mg/L), N40 (0.71 mg/L) and N68 (0.75 mg/L). The variation of chlorine concentration should in part be related to physical characteristics of the pipe material itself and the water age. The same trend was observed in the other simulation runs whose wall decay constant values were $<0.165\ h^{-1}$, In the second simulation run associated with a k_w value of 0.059 h^{-1},

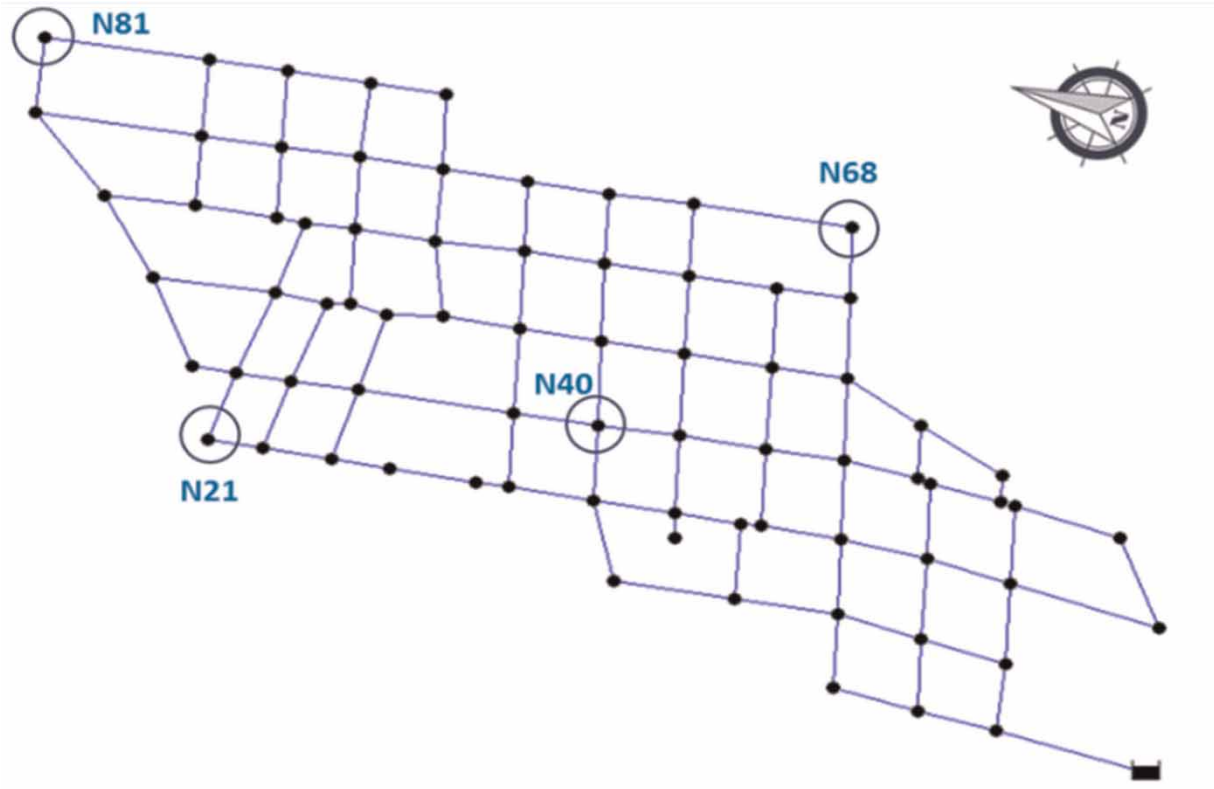

Figure 5 | EPANET model of the San Pedro Nexapa network.

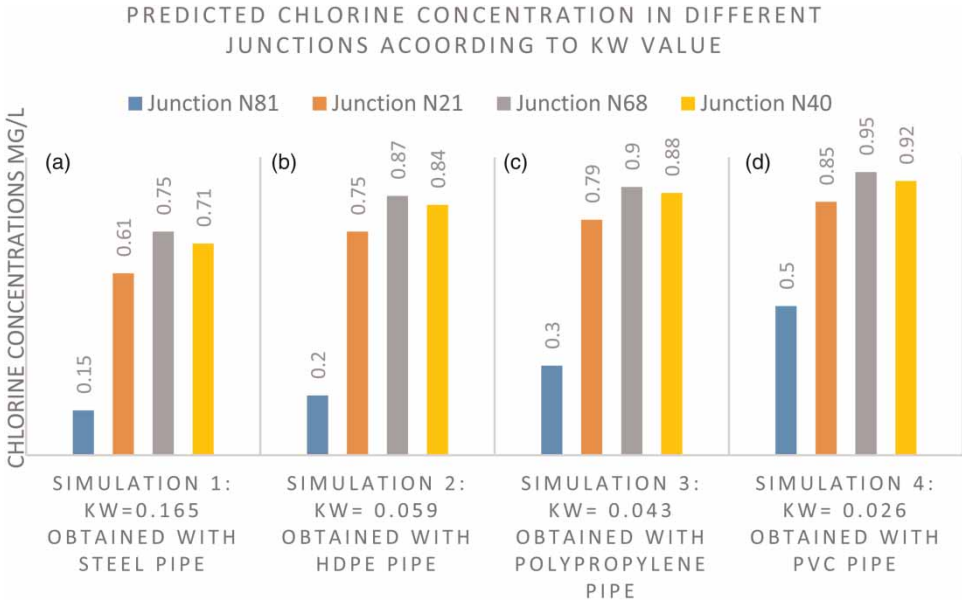

Figure 6 | Predicted chlorine concentration (in four junctions) in the San Pedro Nexapa water distribution network acording to k_w values. (a) $k_w = 0.165\ h^{-1}$, (b) $k_w = 0.059\ h^{-1}$ (c) $k_w = 0.043\ h^{-1}$ and (d) $k_w = 0.026\ h^{-1}$.

results showed slightly lower range of chlorine decay rates than the first run. Chlorine concentrations ranged from 0.20 to 0.87 mg/L. An increase of 0.05, 0.14, 0.12 and 0.13 mg/L was registered in site N81, N21, N68 and N40, respectively. The third and fourth simulation runs were conducted on lower wall decay constants obtained with PP and PVC pipe (0.043 and 0.026 h^{-1} respectively). Consequently higher chlorine concentrations were observed and ranged from 0.30 to 0.90 mg/L and 0.50 to 0.95 mg/L for PP and PVC, respectively and these should be the best materials to rehabilitate the San Pedro Nexapa water distribution network due to their low chlorine demand.

To better understand the impact of the wall friction coefficient on chlorine decay in the network, contour maps of chlorine concentration in the network were created as shown in Figure 7.

In Figure 7(a)–7(c), it is clearly observed that chlorine concentrations of more than 0.25 mg/L was maintained throughout the distribution system. However, chlorine concentration at N81 was below 0.25 mg/L (circled area at the top left corner of the network in Figure 7(d)). The nodes that do not comply with the minimum concentration are located in parts of the branched network furthest point from the reservoir and may be attributed to the water age and the higher wall reaction constant value (0.165 h^{-1}). This result may be because water flow rates are reduced during the hours of lower consumption, increasing the chlorine decay constant and accelerating the decay of the disinfectant Garcíal Avila *et al.* (2021). Chlorine concentrations were under 0.50 mg/L in much larger areas in Figure 7(d) compared to Figure 7(a)–7(c). Junctions N21, N68 and N40 were able to maintain free chlorine concentration above 0.75 mg/L in simulation runs 1, 2 and 3. Therefore, these data confirm the conclusions of Kiéné *et al.* (1998) and Hallam *et al.* (2002), who reported that synthetic materials such as PVC, medium- and high-density polyethylene and PP have a very low chlorine demand. Metallic pipes have high chlorine demand as chlorine reacts with the elemental metal or the associated corrosion products on the pipe wall, especially in metallic pipes.

LIMITATIONS OF THE STUDY

The state of the art of modelling disinfection for chlorine residuals within water distribution systems is typically limited by the uncertainty of reaction coefficients. As with the majority of studies, the design of the current study is subject to limitations such as: the control and analysis of NOM, the low range of chlorine concentration and the use of different pipe diameters in the laboratory than in the field, which may affected the values of the reaction coefficient.

In future studies, it is suggested to run experiments with a higher range of pipe diameters and higher chlorine doses to determine experimental constants. In doing so, it is further necessary to relate these experimental constants to reactant characteristics such as the total organic carbon concentration. These parameters can help in setting the values of the experimental constants during mathematical modelling. In order to fully assess the coefficient obtained in this study and to

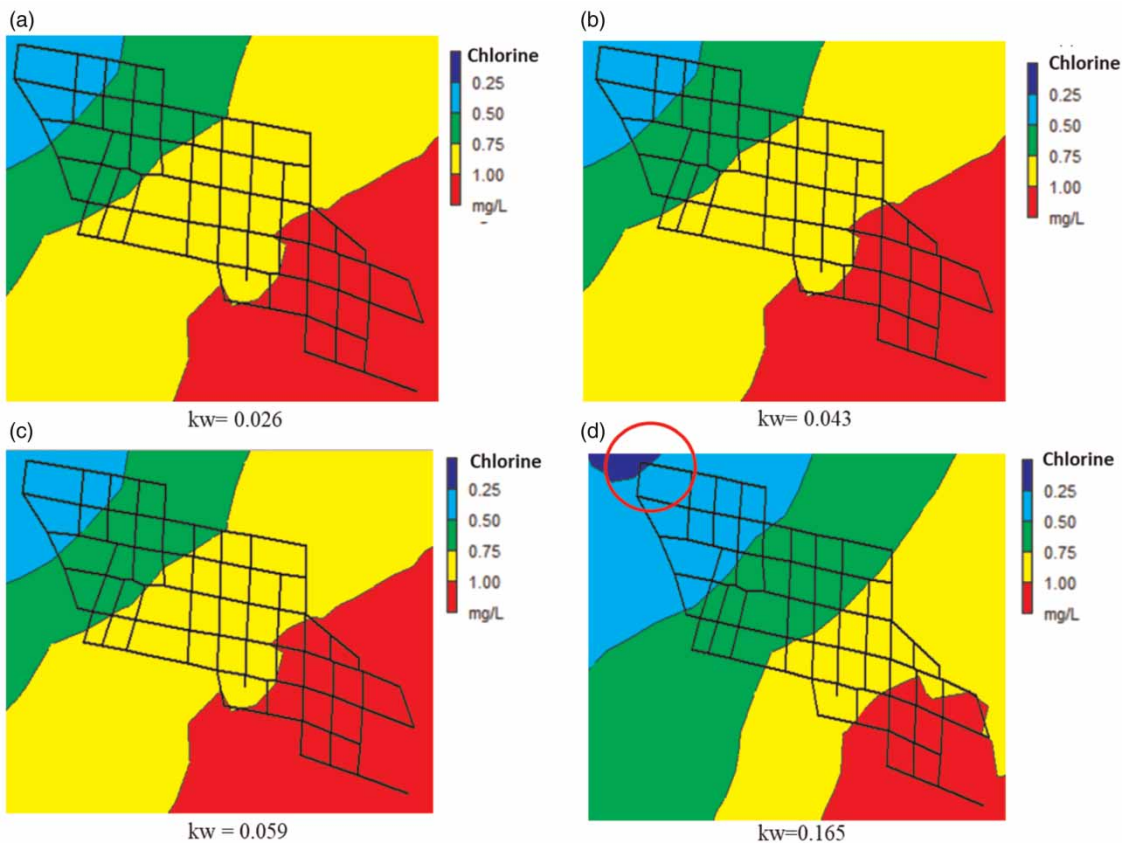

Figure 7 | Simulated chlorine concentrations in the distribution network. (a) When k_w was 0.026 h^{-1}, (b) When k_w was 0.043 h^{-1}, (c) When k_w was 0.059 h^{-1} and (d) When k_w was 0.165 h^{-1}.

determine its limitations for applicability, the model should be further tested in other full-scale water supply systems under different conditions (pipe diameters, chlorine concentration, water age). The model should be calibrated by comparing the predicted and measured chlorine concentration. Finally, to ensure that the mathematical model adequately represents the measured physical phenomena, the root mean square error (RMSE) should be calculated. The optimal value of this parameter is zero, which ensures that the calculated data is identical to the measured value.

CONCLUSIONS

Extended water quality analyses were conducted in a lab set up that consisted four sets of pipes: PVC, GS, PP and HDPE loop pipes of 50 mm in diameter and 12 m in length each. The experiments were performed for two scenarios using initial chlorine doses of 1.21 and 1.60 mg/L. The results revealed the impact of pipe material and initial chlorine concentration on the wall reaction coefficient values. The wall reaction coefficient values were recorded from the highest to the lowest in the following order: GS, HDPE, PP and PVC. This may be explained by the material characteristics of the pipes.

Wall reaction coefficients associated with each pipe material were incorporated in EPANET to predict chorine decay in the San Pedro Nexapa network. Results from this study showed that synthetic material such as especially PVC pipe should be the best option to rehabilitate the San Pedro Nexapa water distribution network because of their lower wall reaction coefficient (k_w) values that implies low chlorine demand of the wall surfaces. In the PVC and PP pipes, higher residual chlorine concentrations were observed that ranged from 0.30 to 0.90 mg/L and 0.50 to 0.95 mg/L, respectively.

The results of this study are useful in understanding the effect of k_w values on chlorine decay and could help develop better management systems to address issues associated with chlorine decay in water distribution systems.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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