

RESEARCH ARTICLE

Chemical disinfection of secondary municipal wastewater effluents: Optimizing CT dose and tailing effects through high-intensity mixing

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Abstract

This paper investigates the impact of average velocity gradient and mixing effects on secondary wastewater coliform inactivation kinetics using an innovative in-line treatment technology based on sodium hypochlorite as disinfecting agent.

Experiments included both laboratory batch kinetic studies (as reference) as well as bench-scale pilot tests. The laboratory studies were carried out using a magnetically stirred vessel to simulate low-mixing conditions ($\bar{G} \approx 1000 \text{ s}^{-1}$ at 1 atm), while the bench-scale pilot tests employed a flow-through system consisting of two centrifugal pumps in series to simulate high average velocity gradients and intense mixing conditions ($\bar{G} \approx 10,000 \text{ s}^{-1}$ at 1.5 atm). In both cases, disinfectant demand and decay models for sodium hypochlorite were fitted against observed data using various expressions corresponding to different kinetic orders and subsequently incorporated into fecal inactivation kinetics via their integral CT expression. Experimental results showed a very remarkable and significant influence of high velocity gradient and mixing intensity on disinfection efficiency. While conventional batch kinetics indicated a 3-log reduction in fecal coliforms at concentration-time integral product (CT) of $16 \text{ (mg} \cdot \text{min} \cdot \text{L}^{-1})$, less than 1/10th of the CT dose (under comparable process conditions) were needed in the case of advanced disinfection with high average velocity gradient and mixing intensity. Using the experimental data collected in this study, a novel inactivation model was developed that uniquely incorporates the average velocity gradient $\bar{G}$ as explicitly kinetic parameter, enabling precise prediction of CT required for various mixing conditions to meet specific microbial treatment targets. To achieve an effluent total coliform concentration of 10 CFU per 100 mL, a CT of $48.5 \text{ mg} \cdot \text{min} \cdot \text{L}^{-1}$ was required at a mixing intensity of $\bar{G} = 762 \text{ s}^{-1}$, while only $0.82 \text{ mg} \cdot \text{min} \cdot \text{L}^{-1}$ was needed at $\bar{G} = 18,158 \text{ s}^{-1}$. Inactivation tailing was drastically reduced

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under high-mixing conditions by enhancing disinfectant penetration in the flocs shielding particle-associated coliforms. Furthermore, disinfection by-product (DBP) screening tests confirmed that enhanced inactivation under high-mixing conditions was achieved while also maintaining regulated DBP levels across all CT values. This integration of mixing effects in microbial inactivation kinetics marks a significant advancement over traditional disinfection design frameworks allowing the disinfection community to access a more refined approach for sizing and validation purposes.

PRACTITIONER POINTS:

- Particle-associated coliforms are inactivated by hypochlorite under high mixing.
- A 3-log reduction of coliforms observed at more than 30 times lower CT under high mixing.
- High mixing and mild pressure can reduce chlorine dose and contact time significantly.
- Tailing effects are well mitigated by high mixing combined with sodium hypochlorite.
- An inactivation model for coliform bacteria accounting for mixing intensity is proposed.

INTRODUCTION

Disinfection is a critical process in wastewater treatment with the aim of reducing the concentrations of microbial pathogens to protect public health. Chemical disinfection using chlorine-based disinfectants is a cost-effective means to achieve microbial inactivation (Luo et al., 2021; Pan et al., 2021; Sun et al., 2021). While chlorine is widely used for its cost-effectiveness and broad-spectrum pathogen inactivation, alternative methods like ozonation, UV, and peracids are also considered because they can reduce disinfection by-product (DBP) formation under certain conditions. Each approach has unique considerations: Ozone provides strong oxidation without chlorinated DBPs, and UV inactivates microbes without chemicals but is limited with high levels of suspended solids. Chlorine remains highly efficient and scalable, and when its drawbacks are managed, it offers a reliable, flexible solution for disinfection in diverse wastewater settings. In hypochlorite-based disinfection, the ClO^- derived from HClO dissolution ($\text{HClO} \leftrightarrow \text{H}^+ + \text{ClO}^-$) and HOCl have a strong oxidation potential and are the key species for microbial inactivation. When applied to wastewater, sodium hypochlorite can react with ammonia to form chloramines as well as with other matrix constituents to form combined chlorine species. As such, to obtain scalable disinfection kinetic parameters, it is important to

relate observed inactivation data to both free and combined chlorine species as they speciate in the wastewater of concern (Audrieth & Rowe, 1955; Berliner, 1931; Guo et al., 2021).

One of the primary concerns with these reactions is production of DBPs, which can have adverse environmental and health effects (Cheng et al., 2023; Helte et al., 2023; Srivastav et al., 2020). The kinetics of DBP formation can vary depending on wastewater quality and contact times, which dictates the chemical dose of a specific disinfectant. Long contact times are usually associated with an increased risk of forming unwanted DBPs. Additionally, certain pathogens may exhibit high resistance to chlorine, requiring high chemical doses or long contact times to achieve the desired inactivation (Wang et al., 2023). For secondary wastewater disinfection, the presence of suspended solids can also hinder microbial inactivation resulting in a phenomenon known as disinfection tailing. In these conditions, the disinfection rate declines over time despite the presence of residual disinfectant, leading to the need for higher doses and extended contact times. (Ge et al., 2021; Ocampo-Rodriguez et al., 2023; Sigstam et al., 2014).

Previous studies have shown that mixing intensity influences chlorination (Samadi et al., 2018; Shodhan & Wei, 2010). White, (1974) reported a consistent pattern illustrating that treatment plants with effective

disinfection systems consistently demonstrated good mixing. Notably, wastewater with high chlorine demand necessitates more efficient mixing to achieve performance comparable to that of wastewater with lower chlorine demand. Improved mixing has also been shown to lead to lower disinfectant residuals (White, 1974), which further reduces dechlorination requirements prior to discharge. Mixing effects are often quantified using the average velocity gradient ($\bar{G}$) parameter, first introduced by Camp and Stein (1943) for coagulation and flocculation studies. From an application standpoint, $\bar{G}$ is a measure of the average rate at which velocity changes in a reference domain, and it is a function of the mechanical power applied to a fluid, the volume of the system being mixed, and the viscosity of the fluid. Lee and Nam (2002) further demonstrated that increasing $\bar{G}$ values during chlorine disinfection, from 0 to 1500 s^{-1} , led to better inactivation of coliforms under atmospheric pressure and room temperature. Specifically, data indicated a logarithmic reduction in total coliforms, with the maximum $\bar{G}$ value of 1500 s^{-1} achieving up to a 5.7 log reduction after 120 min, while without mixing ($\bar{G} = 0$), a 4.9 log reduction was achieved. This highlights that mixing intensity during chemical disinfection can influence disinfection efficiency.

While the importance of mixing during chemical disinfection has been addressed in wastewater disinfection studies, there is a lack of quantitative information, let alone kinetic expression, on the impact of average velocity gradient and mixing intensity on microbial inactivation kinetics associated with $\bar{G}$ values $>1000\text{ s}^{-1}$. These conditions are not necessarily uneconomical for wastewater treatment plants (WWTPs), if we consider that the same can be achieved under mild pressure ($p = 1\text{--}3\text{ atm}$) relining on economical systems such as centrifugal pumps in previous works (Santoro et al., 2013). Moreover, disinfection under high-mixing and mild-pressure conditions could lead to additional synergies such as a better hydraulic efficiency in contacting the disinfectant with the microbial particles, as well as a greater penetration of the chemical favored by mechanisms of disaggregation of the wastewater flocs.

In this paper, we investigated sodium hypochlorite disinfection under both low- and high-mixing conditions in a secondary settled wastewater effluent obtained from a Canadian WWTP located in Ilderton, Ontario. The site was selected because of its reportedly difficult-to-disinfect secondary effluent, with considerable presence of particle-associated coliform bacteria due to the use of aluminum for phosphorus control in the aerated tank and low suspended solids removal efficiency in secondary clarifiers. In this paper, we tested the hypothesis that increasing average velocity gradient mixing intensity,

represented by the velocity gradient ($\bar{G}$), will significantly reduce chlorine demand and microbial inactivation contact time due to enhanced disinfectant penetration is investigated. Additionally, we investigated whether the net effect of disinfecting under high-mixing and mild-pressure conditions would lead to mitigating tailing effects often observed in wastewater disinfection kinetics of unfiltered secondary effluents thus providing a more efficient inactivation process compared to conventional low-mixing methods.

The specific objectives of this study were to compare two different mixing regimes and their impact on disinfection efficiency by the following:

1. Quantifying the impact of mean velocity gradient, $\bar{G}$, on coliform inactivation by sodium hypochlorite in secondary wastewater effluents with high tailing propensity;
2. Assessing the suitability of microbial inactivation kinetics (accounting for disinfectant demand and decay) in predicting disinfection efficiency under various mixing regimes;
3. Developing a novel inactivation model that explicitly accounts for $\bar{G}$ as independent kinetic parameter;
4. Conducting a scenario analysis for chemical dose requirements associated with the novel pilot technology versus conventional systems.

MATERIALS AND METHODS

Secondary effluent wastewater quality

Secondary effluent samples were collected at from the clarifier from a municipal WWTP in Ilderton, Ontario, Canada. This facility employs an extended aeration process to nitrify influent wastewater. An aluminum-based coagulant was dosed in the aeration tank to control phosphorus to $<1\text{ mg}\cdot\text{L}^{-1}$. Samples were collected using sterile containers to prevent microbial contamination and were promptly transported to a laboratory for immediate microbial testing. Conventional wastewater quality parameters were measured for each sample, and results are summarized in Figure 1 and Table S3.

Analytical methods

The analytical methods employed in this study were selected to comprehensively evaluate the disinfection process, focusing on chemical and microbial parameters to assess treatment efficiency, chlorine demand, and the formation of DBPs.

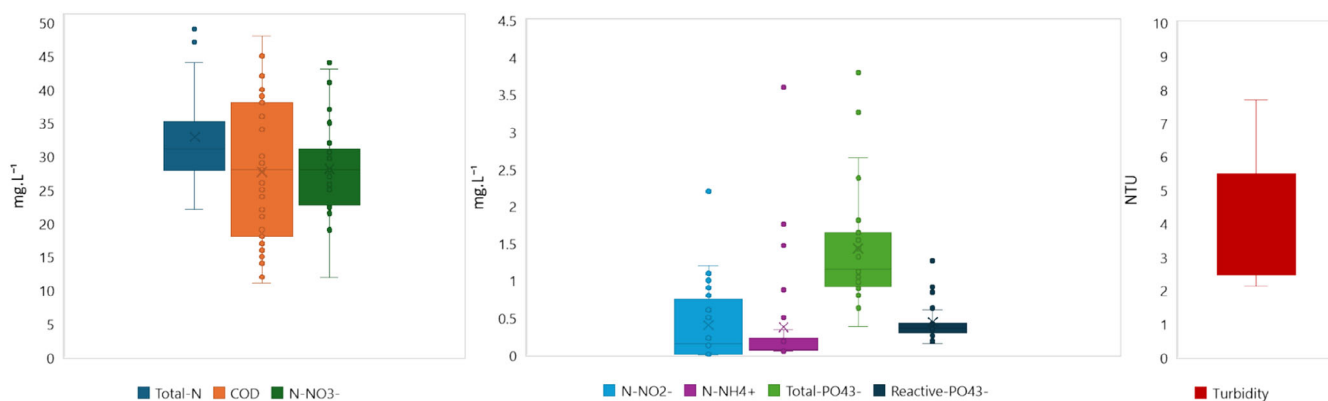


FIGURE 1 Summary of secondary effluent characteristics used for testing.

Chemical analyses

Chemical oxygen demand (COD): COD was determined using Hach Method 8000 (USEPA reactor digestion method), suitable for measurements in the range of 3–150 mg·L⁻¹.

Nitrogen species: Total nitrogen was measured using Hach Method 10,071 (persulfate digestion method), which can measure between 0.5–25 mg·L⁻¹. Ammonia was measured using Hach Method 10,023 (salicylate method) for concentration ranges of 0.02–2.5 mg·N·L⁻¹. Nitrite and nitrate concentrations were determined using Hach methods 10,019 and 10,020, respectively. The former, a diazotization method, can measure between 0.003 and 0.5 mg·N·L⁻¹, while the latter, a chromotropic acid method, is suitable for a range of 0.2–30 mg·N·L⁻¹.

Phosphorus species: Total phosphorus was analyzed using Hach Method 8190 (USEPA PhosVer[®]3 with acid persulfate digestion) suitable for a range of 0.06–3.5 mg·L⁻¹ as PO₄³⁻. Soluble phosphorus was analyzed using the same method, following filtration with a 0.45 µm nylon filter. Reactive phosphorus was evaluated using Hach method 8148 (USEPA PhosVer[®]3 method) suitable for ranges of 0.06–5.0 mg·L⁻¹ as PO₄³⁻.

Chlorine monitoring: During disinfection experiments, total chlorine and free chlorine were immediately determined using Hach Method 8167 and 8021 for total chlorine and free chlorine, respectively. Both methods are suitable for measurements in the range of 0–2 mg·L⁻¹.

All colorimetric tests were conducted using a DR3900 laboratory spectrophotometer from Hach.

DBPs: THMs, HAAs, HANs, HKs, and HALs were extracted and analyzed using liquid–liquid extraction and gas chromatography-electron capture detection, following EPA Methods 551.1 and 552.3.

Microbial analyses

A membrane filtration method was employed for enumeration of total and fecal coliforms with a detection limit of 1 CFU/100 mL. For total coliform, wastewater samples were passed through a 0.45 µm filter and transferred onto mEndo LES agar. Plates were incubated at 35 ± 0.5°C for 18–24 h. Fecal coliforms were measured using Standard Methods for the Enumeration of Water and Wastewater (9222 D), which includes sample filtration through a 0.45 µm filter, which is placed onto mFC agar. Fecal coliforms were incubated at 44.5 ± 0.2°C for 24 ± 2 h.

Conventional batch tests

Sodium hypochlorite, 12.5% W/W aqueous solution was purchased from VWR Chemicals BDH, Canada. For chlorination experiments, stock solutions of sodium hypochlorite were prepared by diluting a commercial solution to 0.1% and measuring the stock concentration using Hach Method 8021 each day before testing.

Microbial inactivation experiments were conducted in a beaker, using a 1000 mL of secondary wastewater effluent. A magnetic stir bar provided gentle mixing at atmospheric pressure and room temperature. Information on the applied conditions and G value calculation for this system is reported in the Supporting Information file. The stock chlorine solution used in the experiment was prepared on the day of the assay using 12.5% w/v sodium hypochlorite and distilled water, and it was stored in a tightly sealed glass bottle. Two sets of conventional batch test experiments were conducted.

In the first set of experiments, varying amounts of sodium hypochlorite were added to the wastewater effluent sample at different chlorine doses (0.4–35.4 mg·L⁻¹,

Table S6). The range of chlorine doses was selected to investigate typical values used for wastewater disinfection (U.S. Environmental Protection Agency (EPA), 1990). These doses were also used to achieve analogous doses in the flow-through pilot in latter experiments. After a constant mixing duration (14, 29 s), samples were collected for water quality analyses. Various contact times were tested to match the conditions achievable in the pilot system, as well as their relevance to full-scale chlorine disinfection systems. Analyses of each sample included: residual chlorine (free and total residual) and total and fecal coliform. Residual chlorine was quenched using sodium metabisulfite at the end of each contact time, prior to coliform measurements.

Based on results of the initial experiments, additional experiments were conducted using different amounts of sodium hypochlorite to mimic varying initial chlorine concentrations (3 and 6 mg·L⁻¹). Following addition of chlorine to the wastewater samples, total chlorine, free chlorine, and total coliform were measured at specific time intervals (2.5, 10, 20, 30, and 40 min) to establish chemical decay rates. Residual chlorine was quenched using sodium metabisulfite at the end of the contact time before total coliform measurement.

Pilot inactivation experiments

This study compares two disinfection systems based on sodium hypochlorite to evaluate the impact of mixing intensity and pressure on microbial inactivation. A

controlled laboratory system to assess low-mixing conditions and a pilot system (Multifunctional Integrated Technology for OXidation of wastewater, commercially known as MITO₃XTM) were used to investigate sodium hypochlorite disinfection. The MITO₃XTM was used because of its ability to provide high-intensity mixing ($\bar{G} > 10,000 \text{ s}^{-1}$) at slightly increased pressure ($p > 1 \text{ atm}$). Of these conditions, high-intensity mixing and increased pressure are expected to mitigate tailing effects by enhancing disinfectant penetration in the flocs otherwise shielding particle-associated coliforms (Zhao et al., 2022). Additionally, the MITO₃X system is anticipated to reduce chlorine losses otherwise encountered in open channel systems (Sander et al., 2022).

The same hypochlorite stock solution used for conventional batch experiments was employed for pilot tests. Pilot disinfection experiments were conducted under high-mixing and mild-pressure conditions using a commercial technology, MITO₃X[®], which is a multifunctional reactor patented by AquaSoil (Fasano, Italy). The technology enables injection of chemical disinfectant between centrifugal pumps in series to provide high mixing ($\bar{G} > 10,000 \text{ s}^{-1}$) under mild pressure ($p = 1\text{--}3 \text{ atm}$). This leads to enhanced contact between the chemical disinfectant and target microbes (Piras et al., 2020; Santoro et al., 2013). The pilot-scale chlorination experiments were conducted in an experimental reactor configuration as shown in Figure 2.

The pilot system consisted of two tanks, each to store untreated and treated wastewater. Undisinfected secondary effluent was fed to the MITO₃X system where

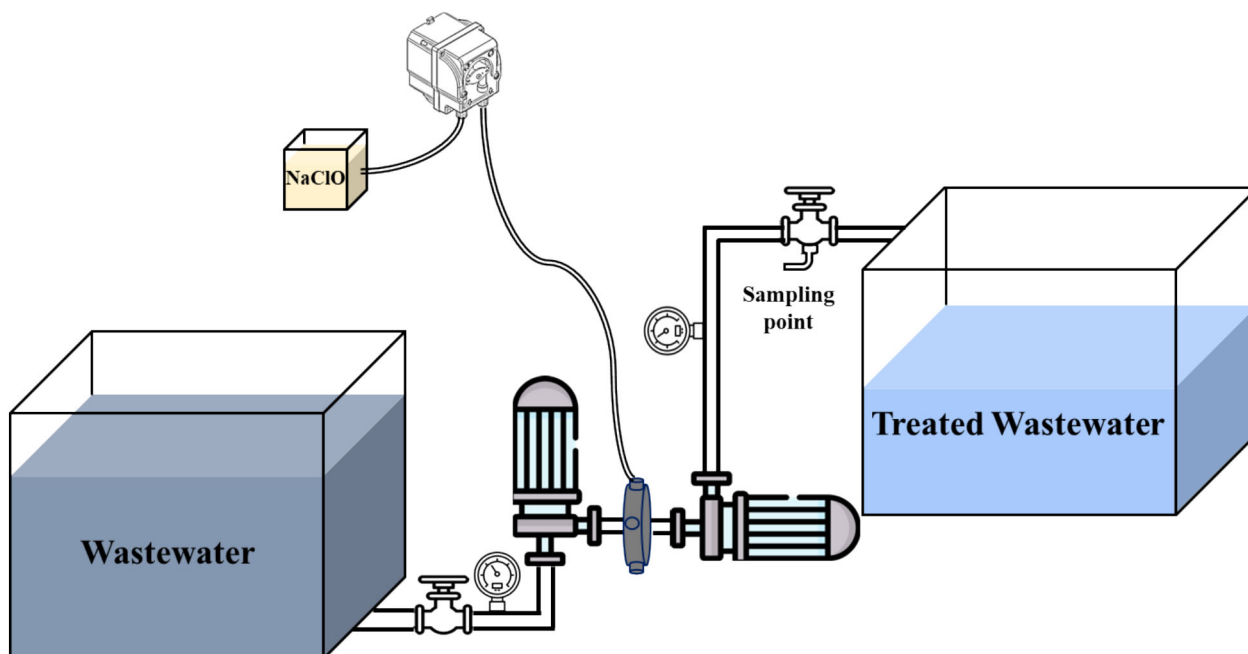


FIGURE 2 Pilot-scale setup used for inactivation experiments under high mixing.

pressure gauges were installed before and after the pumps to determine the applied pressure. Contact time through the MITO₃X was controlled by adjusting a downstream valve. The pump had a maximum output flow of 16–19 L·min⁻¹, with a power output of 10 W and a pump volume of roughly 20 mL. Additional details on experimental conditions are reported in Table S1.

Untreated and treated samples were collected using ports upstream and downstream of the system, respectively. Varying doses of sodium hypochlorite were injected to achieve the desired initial concentration of the disinfectant using a precision flow peristaltic pump, calibrated before testing. The hypochlorite stock solution was generated daily, and initial sodium hypochlorite concentration measured before the test. The mean velocity gradient $\bar{G}$ for mechanical mixing expressed in units of s⁻¹ was calculated as shown in Equation (1).

$$\bar{G} = \sqrt{\frac{P_{Elect} \times \eta}{\mu \times V}} \quad (1)$$

where P_{Elect} is electrical power input expressed in units of N·m·s⁻¹ (W) and η is the efficiency of the pump. μ is absolute water dynamic viscosity (N·s·m⁻²) which for water at 15°C is 0.0011373 N·s·m⁻², and V is volume of basin (m³).

Experiments were conducted by adjusting flows to 3.7 and 12 L·h⁻¹; the speed of the peristaltic pump for injecting the sodium hypochlorite solution was operated at six different speeds (0, 10, 20, 40, 80, and 120 rpm) to achieve conditions reported in Table S5. The overall calculated $\bar{G}$ value (Equation (1)) for this system is 18,158 s⁻¹ and pressure was 1.48 atm. More information on $\bar{G}$ value estimation is reported in the Supporting Information file.

Using the effluent ports shown in Figure 2, samples were collected for analysis. The analyses included immediate measurement of residual chlorine (both free and total chlorine), and following quenching of the residual using sodium metabisulfite and total and fecal coliform were analyzed.

Tracer tests were performed to determine the actual contact time between disinfectant and secondary effluent wastewater. For this purpose, methylene blue solution was injected at various peristaltic pump speeds into the upstream of the MITO₃X system. Samples were collected every 30 s from the MITO₃X system outlet at sampling point (shown in Figure 2) and analyzed for by measuring sample absorbance at a wavelength of 665 nm. The t_{10} (time at which 10% of the methylene blue reached the effluent port) was used in the dose calculations.

Model development

Inactivation kinetics were modeled under different mixing regimes, which is essential to development of advanced chemical disinfection control for meeting microbial inactivation objectives at WWTPs (Cao et al., 2021; Manoli et al., 2019). Numerous models have been developed to describe disinfectant demand and decay (Manoli et al., 2019; Santoro et al., 2007; Santoro et al., 2015; Sarathy et al., 2016). Some studies propose empirical equations (Cerf, 1977; Chick, 1908; Hom, 1972), while others, like the model presented in Severin et al. (1983), have developed equations from first principles. Still, a knowledge gap exists for quantitative inactivation models that explicitly incorporate effects of mixing on microbial inactivation kinetics.

Disinfectant decay models

When disinfectant is added to a disinfection contact tank, it interacts with organic and inorganic substances. This interaction leads to a reduction in the chlorine concentration from its initial concentration at the point of dosing. There are several models that describe this disinfectant decay process and selection of an appropriate numerical model is important due to the practical impossibility of obtaining a comprehensive multivariate distribution that governs disinfection. The complexity of wastewater disinfection, with its myriad factors and latent variables, compounds this challenge. In this study, we present and compare nine disinfectant decay models to elucidate the dynamics of the process. The simplest of these, the first-order decay model, is used to describe disinfectant decay in wastewater and is detailed in Equation (2).

$$C_t = C_0 \times \exp(-kt) \quad (2)$$

The concentration of the disinfectant C_t (mg·L⁻¹), at a specific time, t (min) is determined by the initial concentration of the disinfectant, C_0 (mg·L⁻¹), and the first-order rate constant, k (min⁻¹). However, it does not reflect an initial decay when disinfectant is introduced into wastewater; thus, to capture this instantaneous demand (D), followed by a first-order decay (k), the following relationship can be used, as outlined in Equation (3).

$$C_t = (C_0 - D) \times \exp(-kt) \quad (3)$$

The initial demand for the disinfectant is determined by D (mg·L⁻¹).

The third model proposes a different approach to instantaneous demand (D), suggesting it is represented by dimensionless value, α , multiplied by the initial dose of the disinfectant (C_0), as shown in Equation (4).

$$C_t = (C_0 - (\alpha \times C_0)) \times \exp(-kt) \quad (4)$$

In the fourth model, chlorine decay is depicted as a combination of two first-order kinetics reactions, as illustrated in Equation (5).

$$C_t = C_{01} \times \exp(-k_1 t) + C_{02} \times \exp(-k_2 t) \quad (5)$$

where k_1 and k_2 are first-order rate constants (min^{-1}) and C_{01} and C_{02} are modeled initial disinfectant concentrations ($\text{mg} \cdot \text{L}^{-1}$).

Disinfection is complex, involving multiple reactions and factors that can complicate its kinetics. First-order models may not accurately capture all aspects of these processes, particularly when they exhibit behaviors such as tailing or shouldering. To address these effects, a second-order kinetic model was applied, as shown in Equation (6).

$$\frac{1}{C_t} - \frac{1}{C_0} = kt \quad (6)$$

Like the first-order model, this model was developed using instantaneous demand (D) and α , as shown in Equations (7, 8).

$$\frac{1}{C_t} - \frac{1}{C_0 - D} = kt \quad (7)$$

$$\frac{1}{C_t} - \frac{1}{C_0 - (\alpha \times C_0)} = kt \quad (8)$$

The integral estimate of the time-dependent residual disinfectant concentration (CT dose in $\text{mg} \cdot \text{min} \cdot \text{L}^{-1}$), defined as the area under the disinfectant decay curve, is provided by Equations (9–15). These equations correspond to kinetics models of Equation (2–8), respectively.

$$CT = \frac{C_0}{k} \times (1 - e^{(-kt)}) \quad (9)$$

$$CT = \frac{(C_0 - D)}{k} \times (1 - e^{(-kt)}) \quad (10)$$

$$CT = \frac{C_0 - (\alpha \times C_0)}{k} \times (1 - e^{(-kt)}) \quad (11)$$

$$CT = \frac{C_{01}}{k_1} \times (1 - e^{(-k_1 t)}) + \frac{C_{02}}{k_2} \times (1 - e^{(-k_2 t)}) \quad (12)$$

$$CT = \frac{1}{k} \times \ln \left(kt + \frac{1}{C_0} \right) - \frac{1}{k} \times \ln \left(\frac{1}{C_0} \right) \quad (13)$$

$$CT = \frac{1}{k} \times \ln \left(kt + \frac{1}{(C_0 - D)} \right) - \frac{1}{k} \times \ln \left(\frac{1}{(C_0 - D)} \right) \quad (14)$$

$$CT = \frac{1}{k} \times \ln \left(kt + \frac{1}{(C_0 - (\alpha \times C_0))} \right) - \frac{1}{k} \times \ln \left(\frac{1}{(C_0 - (\alpha \times C_0))} \right) \quad (15)$$

Integral CT-based microbial inactivation kinetics models

The initial inactivation of microbes is typically rapid, followed by a slower inactivation phase due to the microbes being shielded by particles where they are aggregated. This results in tailing: an effect of microbes being effectively protected from the chemical disinfectant. This biphasic behavior of microbial inactivation in wastewater can be represented by a double-exponential model, which is the sum of two exponential terms, each representing one of the two phases (Cerf, 1977; Santoro et al., 2007), as shown in Equation (16).

$$N_{(CT)} = N_0 \times \beta \times e^{-k_d \times CT^m} + N_0 \times (1 - \beta) \times e^{-k_p \times CT} \quad (16)$$

In this equation, N_0 and $N_{(CT)}$ represent the initial and final concentrations (after treatment) of culturable microbes, respectively, measured in colony-forming units (CFU) per 100 mL. The variable β stands for the fraction of particle-associated particles. The terms k_d and k_p are the CT dose-dependent inactivation rate constants for dispersed and particle-associated microbes, respectively. They are measured in units of $(\text{L} \cdot \text{mg}^{-1} \cdot \text{min}^{-1})^m$ and $\text{L} \cdot \text{mg}^{-1} \cdot \text{min}^{-1}$. A parameter, m , which has been introduced into the first exponent of the double-exponential model illustrates tailing ($m < 1$) or shouldering ($m > 1$) (Haas & Joffe, 1994).

An alternative model suggests that disinfection is affected by mixing intensity ($\bar{G}$). To consider the $\bar{G}$ effect, the well-known microbial inactivation model is enhanced, as shown by Equation (17).

$$N_{(CT)} = N_0 \times \beta \times e^{-k_d \times \bar{G}^{r1} \times CT^m} + N_0 \times (1 - \beta) \times e^{-k_p \times \bar{G}^{r2} \times CT} \quad (17)$$

CT, measured in $\text{mg} \cdot \text{min} \cdot \text{L}^{-1}$, are integral estimates of the time-dependent residual concentrations of chlorine

species. The variables k_d and k_p , expressed in units of $(\text{L}\cdot\text{mg}^{-1}\cdot\text{min}^{-1})^m$ and $\text{L}\cdot\text{mg}^{-1}\cdot\text{min}^{-1}$ represent the CT dose-dependent inactivation rate constants for dispersed and particle-associated microbes, respectively. γ_1 and γ_2 are $\bar{G}$ effects corrections.

To provide perspective on model performance and elucidate strengths and weaknesses of predictive models, several statistical parameters need to be calculated. R -squared (R^2) indicates how well the data fit the regression model. Root mean squared error (RMSE) is an indicator of the accuracy of a regression model in predicting data points within a dataset. A lower RMSE value indicates a better fit of the model to the data, meaning the predicted values are closer to the observed values. The Bayesian information criterion (BIC) is another statistical measure used for model selection. The BIC is based on a likelihood function and includes a penalty term for the

number of parameters in the model to avoid overfitting. When comparing models, a lower BIC is generally preferred suggesting a balance between model complexity and data fit.

RESULTS AND DISCUSSION

During batch testing, changes in total and free chlorine were monitored during 40 min of low mixing ($G = 762 \text{ s}^{-1}$) and atmospheric pressure (Figure 3a,b); experimental conditions and results are summarized in Table S4. In the initial 2.5 min, free chlorine dropped steadily from 3 to $0.16 \text{ mg}\cdot\text{L}^{-1}$, and from 6 to $0.38 \text{ mg}\cdot\text{L}^{-1}$, indicating that free chlorine is dominant at the start of the disinfection process. With respect to total chlorine, there was a decrease of 0.81 and $0.64 \text{ mg}\cdot\text{L}^{-1}$ in

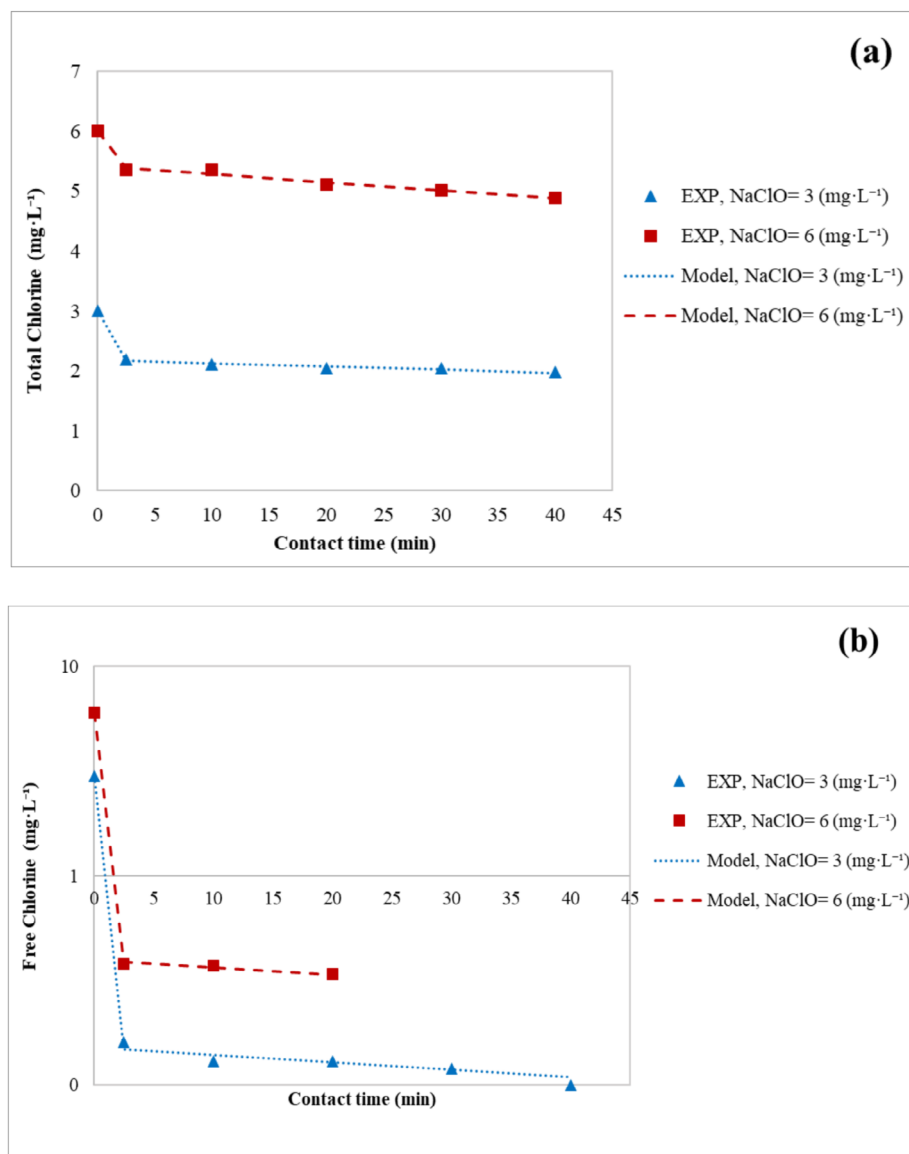


FIGURE 3 The experimental data and disinfectant decay model's predictions for residual total chlorine concentration (a), and free chlorine concentration (b) as a function of time for initial concentrations of 3 and $6 \text{ mg}\cdot\text{L}^{-1}$ over low mixing and atmospheric pressure.

the first 2.5 min, and a decrease of 0.21 and 0.48 mg·L⁻¹ in the subsequent 37.5 min for 3 and 6 mg·L⁻¹ NaClO doses, respectively. These findings suggest the majority of disinfectant decay and microbial inactivation occur at the beginning of the process, prompting further investigation into shorter time frames.

The study on disinfection was expanded and conducted over high mixing ($\bar{G} = 18,158 \text{ s}^{-1}$) and high-pressure regime using the pilot system. Experimental conditions and results for pilot testing, along with the analogous batch testing experiments, are shown in Tables S5 and S6. Results show that the high-mixing, mild-pressure regime demonstrated a lower chlorine demand compared to the low mixing, atmospheric pressure regime. With a chlorine dose of 1.4 mg·L⁻¹, the residual chlorine observed in the flow-through MITO₃X system was higher than that in analogous batch tests. This disparity was more apparent at higher chlorine doses, and this trend was consistent across all the chlorine doses tested. These observations imply that the high mixing, pressured regime could provide benefits in terms of chlorine consumption and effectiveness.

Under the low mixing, atmospheric pressure regime, both total and fecal coliforms were only partially inactivated under all experimental conditions. However, when using the high mixing and pressured regime, complete inactivation was observed, even with lower doses of NaClO. This underscores the impact of mixing intensity on microbial inactivation. When comparing mixing regimes, considering mixing intensity, it is worth noting that in the batch system, the velocity gradient ($\bar{G} = 762 \text{ s}^{-1}$) was lower than in the flow-through system ($\bar{G} = 18,158 \text{ s}^{-1}$). Mean velocity gradient ($\bar{G}$) calculations for each system are detailed in the supplementary materials. Experimental findings suggest intense mixing could enhance disinfection efficiency.

Disinfectant decay models evaluation

The disinfectant decay models were fitted using two different initial concentrations of NaClO and varying contact times up to 40 min for the low-mixing case at atmospheric pressure. Table 1 provides a summary of the adjusted parameters for the nine disinfectant decay models (Equations 2–8) based on residual concentrations of free and total chlorine. The Microsoft Excel Solver was used for modeling the data, and the parameters were identified by minimizing the sum of squared errors between observed and modeled chlorine residual data. The best fit model was selected jointly considering three statistical parameters, namely, the *R*-squared (*R*²), BIC, and RMSE.

The most accurate model, in all circumstances, was that having two first-order kinetic parameters; the first describing the rapid disinfectant consumption due to nearly instantaneous chlorine demand and the second describing slow decay. Figure 3a,b depicts these predictions for both free and total chlorine as a function of time for doses of 3 and 6 mg·L⁻¹. The predicted *k*₁ and *k*₂ values for free and total chlorine (where *k*₁ > *k*₂) quantitatively confirms that the disinfectant decay follows a fast regime initially and transitions to slower first-order kinetics over low mixing and atmospheric pressure regime. After choosing the optimum model, the CT value was calculated accordingly to serve for microbial inactivation prediction.

The same parameter estimation procedure was applied to the pilot testing scenarios, with results shown in Tables S7 and S8, respectively. In the case of total chlorine, the estimated rapid chlorine demand was higher for the low-mixing regime, suggesting that more chlorine losses were experienced in a vessel open to atmospheric pressure. This may be related to two factors: first, high mixing can mitigate disinfectant losses by preventing hot-spots of poorly mixed regions within the fluid volume of concern. Secondly, the enclosed pilot reactor used for high-mixing experiments, as described in literature (Piras et al., 2020; Santoro et al., 2013), may prevent losses due to chlorine volatilization. A third potential explanation may be that high-mixing conditions in the continuous flow MITO₃X system provide higher turbulent dispersion. Figure S1 reports the measured free chlorine after high and low mixing.

In terms of the decay rate constant (*k*), the low mixing, atmospheric pressure batch tests had a much higher decay rate (1.36E-01 min⁻¹) than the high mixing, pressured pilot tests (7.29E-03 min⁻¹). The higher rate constant in batch mixing implies a quicker decay of chlorine, meaning that chlorine is consumed faster than in a high-mixing regime. Conversely, the lower rate constant in the pilot system allows chlorine to persist longer, enhancing its disinfection effectiveness.

Integral CT-based microbial inactivation model evaluation

Figure 4 represents the normalized concentration (*N*/*N*₀) of total coliform versus CT, for the batch testing scenarios, based on total chlorine concentrations. The corresponding figure using free chlorine residuals is provided as Figure S2. The data and model fit were derived from experimental observations and a mathematical model (Equation 16), respectively. Inactivation of total coliform over time was linear with tailing (Ocampo-Rodriguez

TABLE 1 Fitted parameters of proposed disinfectant decay models, their performance metrics over low mixing.

Total chlorine				Free chlorine				
Chlorine decay model	Model parameters	R ²	RMSE (mg·L ⁻¹)	BIC	Model parameters	R ²	RMSE (mg·L ⁻¹)	BIC
$C_t = C_0 \times \exp(-kt)$	k (min ⁻¹): 7.66E - 03	9.57E - 01	4.15E - 01	-1.86E + 01	k (min ⁻¹): 1.12E + 00	9.96E - 01	1.76E - 01	-3.24E + 01
$C_t = (C_0 - D) \times \exp(-kt)$	D (mg·L ⁻¹): 7.61E - 01 k (min ⁻¹): 1.71E - 03	9.98E - 01	9.78E - 02	-5.08E + 01	D (mg·L ⁻¹): 8.48E - 01 k (min ⁻¹): 1.04E + 00	9.96E - 01	1.76E - 01	-3.01E + 01
$C_t = (C_0 - (a \times C_0)) \times \exp(-kt)$	k (min ⁻¹): 2.65E - 03 Alfa: 1.3E - 01	9.92E - 01	2.92E - 01	-2.46E + 01	k (min ⁻¹): 1.23E - 02 Alfa: 9.35E - 01	1.00E + 00	2.37E - 02	-7.03E + 01
$\frac{1}{C_t} - \frac{1}{C_0} = kt$	k (min ⁻¹): 1.48E - 03	9.53E - 01	4.96E - 01	-1.43E + 01	k (min ⁻¹): 1.03E + 00	9.95E - 01	1.47E - 01	-3.60E + 01
$\frac{1}{C_t} - \frac{1}{C_0 - D} = kt$	D (mg·L ⁻¹): 8.15E - 01 k (min ⁻¹): 2.38E - 04	9.97E - 01	1.15E - 01	-4.70E + 01	D (mg·L ⁻¹): 2.75E + 00 k (min ⁻¹): 6.5E - 01	9.97E - 01	1.25E - 01	-3.70E + 01
$\frac{1}{C_t} - \frac{1}{C_0 - (a \times C_0)} = kt$	k (min ⁻¹): 1.3E - 04 Alfa: 1.66E - 01	9.88E - 01	3.17E - 01	-2.26E + 01	k (min ⁻¹): 2.67E - 02 Alfa: 9.39E - 01	1.00E + 00	3.34E - 02	-6.34E + 01
$C_t = C_{01} \times \exp(-k_1 t) + C_{02} \times \exp(-k_2 t)$	k ₁ (min ⁻¹): 6.48E + 00 C ₀₁ (mg·L ⁻¹): 8.14E - 01, 5.68E - 01 k ₂ (min ⁻¹): 2.65E - 03 C ₀₂ (mg·L ⁻¹): 2.19E + 00, 5.43E + 00	1.00E + 00	2.84E - 02	-7.06E + 01	k ₁ (min ⁻¹): 8.08E + 00 C ₀₁ (mg·L ⁻¹): 2.85E + 00, 5.6E + 00 k ₂ (min ⁻¹): 8.17E - 03 C ₀₂ (mg·L ⁻¹): 1.51E - 01, 3.96E - 01	1.00E + 00	6.47E - 03	-8.70E + 01

Abbreviations: BIC, Bayesian information criterion; RMSE, root mean squared error.

et al., 2023; Owoseni et al., 2017) with the initial inactivation of dispersed microbes occurring quickly. This linear response is followed by a slower inactivation phase, attributed to particle-associated microbes. The CT was calculated using Equation (12), with parameters fitted from the best disinfectant decay model (selected by previous discussion), for free and total chlorine. These calculated CTs were used in Equation (16) to fit microbial inactivation data. Model parameters were optimized using Excel Solver to minimize the sum of squared errors between observed and predicted total coliform after treatment. Fitted parameters, and statistical indices are presented in Table S9. Based on the fitted parameters of the microbial inactivation model, the β -value was

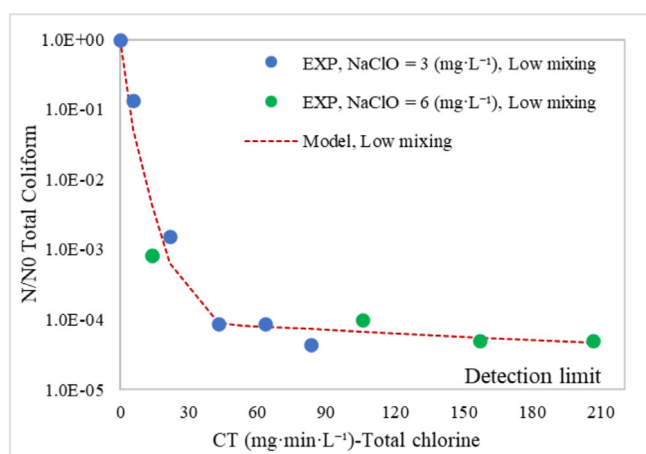


FIGURE 4 Evaluation of the experimental data and microbial inactivation model over low mixing ($\bar{G} = 762 \text{ s}^{-1}$) based on total chlorine; contact times to generate CTs ranged from 0 to 40 min.

approximately 1, suggesting the proportion of dispersed microbes is greater than particle-associated microbes. This could have significant implications for disinfection, as dispersed microbes might respond differently to treatment compared to particle-associated microbes.

Figures 5 and 6 display the normalized concentration (N/N_0) of total and fecal coliforms against CT based on total chlorine, respectively. The same figures for CT based on residual free chlorine are shown in Figure S3, and Figure S5, for total and fecal coliform, respectively. These figures illustrate inactivation of coliforms in under both high- (pilot testing) and low-mixing (bench testing) regimes, as determined by experimental data and a mathematical model (Equation 16). The CT was calculated with parameters derived from a first-order disinfectant decay model (Equation 3) for free and total chlorine. Results revealed a strong correlation between observed and model predicted microbial inactivation data in both mixing regimes.

Results showed a downward trend in inactivation rates for both experimental and model data, indicating that as the CT increases, the normalized concentration (N/N_0) of coliform species decreases. However, the rate of inactivation varies between conditions. The low mixing, atmospheric pressure regime showed a less steep slope compared to the high mixing, pressurized regime. This suggests inactivation occurred at a slower rate under low mixing, atmospheric pressure conditions. This difference in inactivation rates can be attributed to the enhanced penetration of disinfectant inside the wastewater particles, or to a higher exposure of bacteria to more disinfectant enabled by high mixing. While this interpretation provides a general understanding of the trends and

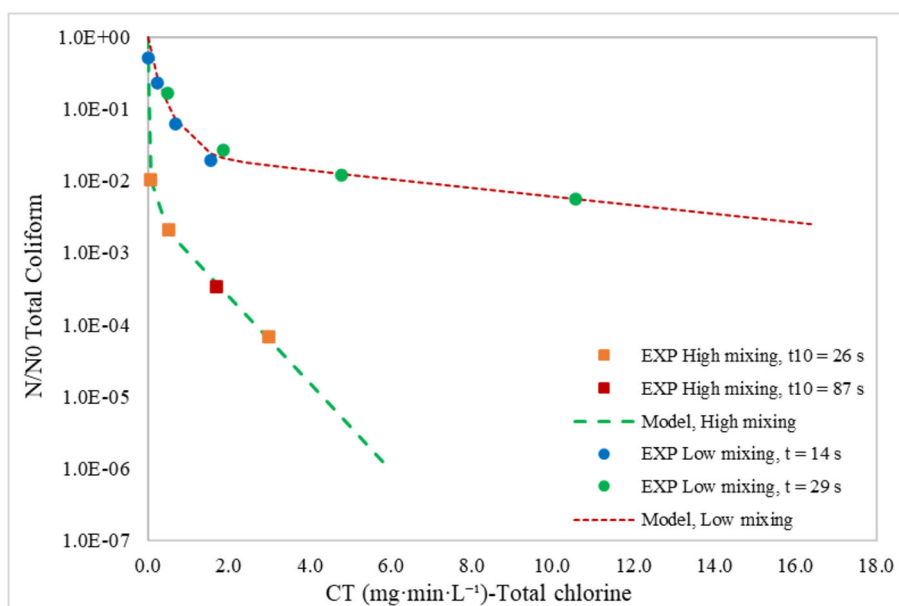


FIGURE 5 Evaluation of total coliform inactivation models over high mixing ($\bar{G} = 18,158 \text{ s}^{-1}$) and low mixing ($\bar{G} = 762 \text{ s}^{-1}$) based on total chlorine; NaClO concentrations to generate CTs ranged from 0.4 to 35.4 $\text{mg}\cdot\text{L}^{-1}$.

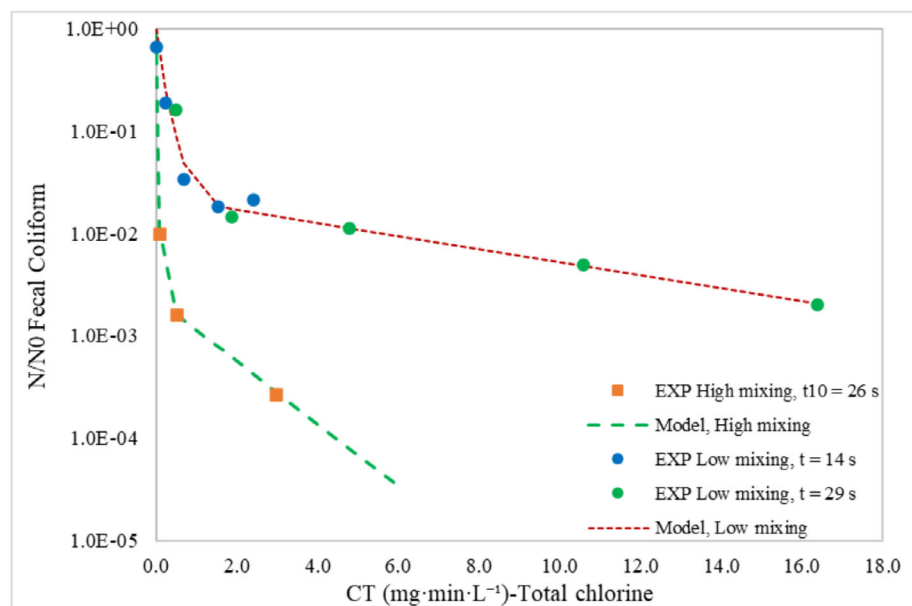


FIGURE 6 Evaluation of fecal coliform inactivation models over high mixing ($\bar{G} = 18,158 \text{ s}^{-1}$) and low mixing ($\bar{G} = 762 \text{ s}^{-1}$) based on total chlorine; NaClO concentrations to generate CTs ranged from 0.4 to $35.4 \text{ mg} \cdot \text{L}^{-1}$.

relationships in the data, a comprehensive assessment of these mechanisms requires additional investigations with methods outside the scope of this paper.

Model parameters were optimized, and the optimized parameters, along with associated statistical measures such as R -squared (R^2), BIC, and RMSE, are presented in Tables S10 and S11 for total coliform and fecal coliform, respectively. The model adjusted parameters revealed that the β -value was ~ 1 in both mixing regimes, suggesting a higher proportion of dispersed microbes compared to particle-associated microbes. The m parameter in low mixing was < 1 for both total and fecal coliform, indicating a shoulder effect in the dose–response kinetics. This implies the rate of microbial inactivation does not decrease proportionally with increasing CT; instead, at low CT, it increases suggesting a diffusion limitation associated with the penetration of the disinfecting species in the wastewater flocs. This is further supported by the m parameter, which was > 1 , a finding consistent for both total and fecal coliform. These results indicate that high mixing, pressured conditions can achieve microbial inactivation in a shorter contact time and with less chlorine. Further, the fitted k_d and k_p values under high mixing, pressured conditions were approximately tenfold higher than in low mixing, further confirming rapid microbial inactivation under these conditions (Table S10, Table S11).

The enhanced model was evaluated to assess mixing regimes by considering $\bar{G}$. The model suggested that disinfection efficiency varies with the $\bar{G}$ value. Both batch and pilot data were fitted by Equation 17. CT was calculated, and $\bar{G}$ differs according to each mixing regime with G values of 762 and $18,158 \text{ s}^{-1}$ for low- and high-mixing

regimes, respectively. After model evaluation, two other $\bar{G}$ values were applied. Figures 7 and 8 display normalized concentration (N/N_0) of total and fecal coliforms against CT, respectively. The same figures for CT based on free chlorine are shown in Figures S5 and S6, for total and fecal coliform, respectively. These figures illustrate inactivation of coliforms under several velocity gradients ($\bar{G}$), as determined by experimental data and the enhanced model (Equation 17). Results reveal good correlation between observed and predicted microbial inactivation data. Model parameters were optimized for microbial indicators and are presented with statistical metrics in Table 2 for total and fecal coliform.

The microbial inactivation model consistent shows $\gamma_2 > \gamma_1$, which indicates that mixing intensity, $\bar{G}$, has a more pronounced impact on particle-associated microbes than dispersed microbes. This distinction is important because particle-associated microbes are often shielded by particulates, making them less accessible to the disinfectant and thus more resistant to disinfection. The higher effect of mixing intensity ($\bar{G}$) on particle-associated microbes compared to dispersed microbes aligns with our initial hypothesis, which posited that mixing intensity plays a significant role in mitigating disinfection tailing effects associated with suspended solids.

Based on the fitted parameters for total chlorine, the microbial models for total and fecal coliforms as a function of N_0 , CT, and $\bar{G}$ follow:

$$N_{\text{total coliform}(CT)} = N_0 \times 0.076 \times e^{-0.049 \times \bar{G}^{0.463} \times CT^{0.36}} + N_0 \times 0.924 \times e^{-0.0006 \times \bar{G}^{1.356} \times CT} \quad (18)$$

FIGURE 7 Evaluation of total coliform inactivation models over several mixing intensity, based on total chlorine; NaClO concentrations to generate CTs ranged from 0.4 to 35.4 mg·L⁻¹.

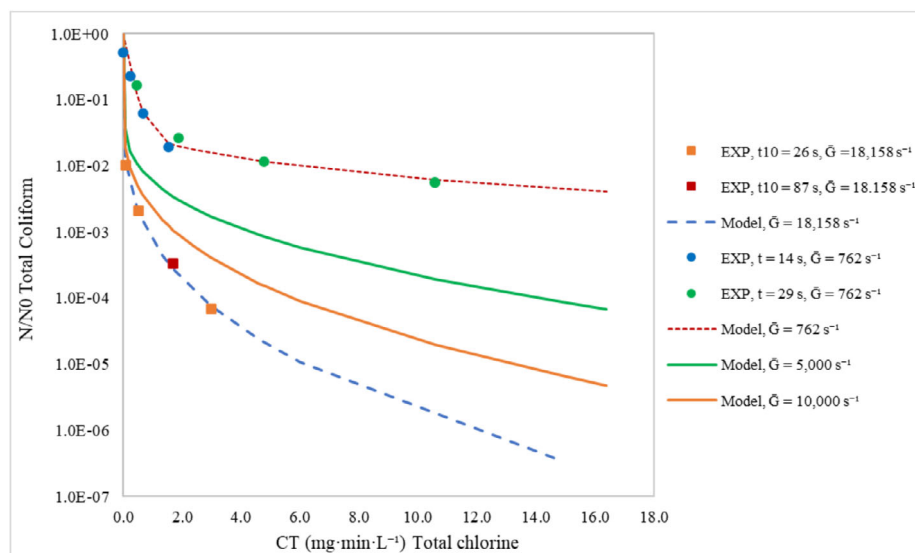
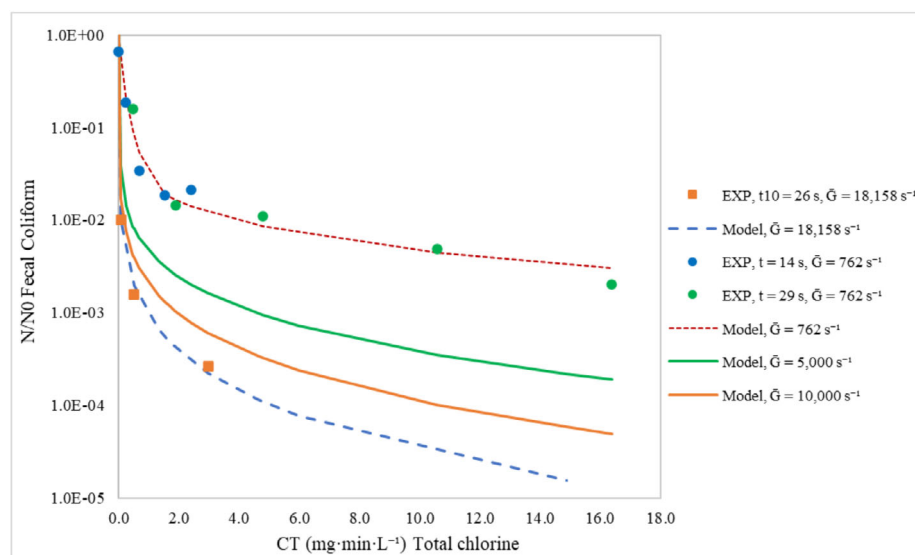


FIGURE 8 Evaluation of fecal coliform inactivation models over several mixing intensity, based on total chlorine; NaClO concentrations to generate CTs ranged from 0.4 to 35.4 mg·L⁻¹.



$$N_{Fecal\ coliform(CT)} = N_0 \times 0.521 \times e^{-0.677 \times \bar{G}^{0.228} \times CT^{0.184}} + N_0 \times 0.479 \times e^{-0.0009 \times \bar{G}^{1.285} \times CT} \quad (19)$$

Integral CT dose requirements for different mixing and velocity gradients

There are several wastewater disinfection regulations and guidelines that require high-level disinfection, such as in water reuse applications (U. US EPA, 2012). Treatment objectives can vary depending on the intended use of the recycled water (Shoushtarian & Negahban-Azar, 2020). For example, reclaimed water used for irrigation may have different limits compared to reclaimed water that is

used for industrial cooling (Jaramillo & Restrepo, 2017). In any case, these limits are typically based on indicator organisms that suggest the presence of potentially harmful microbes. For instance, in California, recycled water for irrigation must have total coliform <2.2 CFU/100 mL (U. US EPA, 2012).

To demonstrate practical use of the model, several scenarios have been assessed (<1000, 100, and 10 CFU/100 mL of total and fecal coliforms). For this purpose, CT values were predicted to meet each target using the model for each mixing regime. For this scenario analysis, a contact time of 60 min was assumed using the low-mixing regime to simulate a traditional chlorine contact tank, while 30 s contact time was assumed for the high-mixing regime MITOX system (i.e., the time

TABLE 2 Microbial inactivation model (Equation 17) parameters and performance metrics for both mixing regimes.

Model parameters	Total coliforms				Fecal coliforms			
	R^2	BIC	RMSE (mg·L ⁻¹)		R^2	BIC	RMSE (mg·L ⁻¹)	
Total chlorine	β : 0.076 m : 0.36 γ_1 : 0.463 γ_2 : 1.356 k_d (L·mg ⁻¹ ·min ⁻¹) ^m : 0.049 k_p (L·mg ⁻¹ ·min ⁻¹): 0.0006	9.47E – 01 – 1.14E + 02	1.00E – 01	Total chlorine	β : 0.521 m : 0.184 γ_1 : 0.228 γ_2 : 1.285 k_d (L·mg ⁻¹ ·min ⁻¹) ^m : 0.677 k_p (L·mg ⁻¹ ·min ⁻¹): 0.0009	9.70E – 01 – 1.06E + 02	1.15E – 01	
Free chlorine	β : 0.167 m : 0.3003 γ_1 : 0.381 γ_2 : 1.36 k_d (L·mg ⁻¹ ·min ⁻¹) ^m : 0.135 k_p (L·mg ⁻¹ ·min ⁻¹): 0.0006	7.67E – 01 – 3.62E + 01	5.05E – 01	Free chlorine	β : 0.527 m : 0.179 γ_1 : 0.228 γ_2 : 1.34 k_d (L·mg ⁻¹ ·min ⁻¹) ^m : 0.686 k_p (L·mg ⁻¹ ·min ⁻¹): 0.0006	7.59E – 01 – 3.53E + 01	4.99E – 01	

Abbreviations: BIC, Bayesian information criterion; RMSE, root mean squared error.

TABLE 3 Predicted CT value and initial NaClO concentration required to meet specific limits for both total and fecal coliform with initial concentration of 10^4 CFU/100 mL.

Process	Total coliform				Fecal coliform			
	Microbial limit (CFU/100 mL)	Predicted CT ($\text{mg}\cdot\text{min}\cdot\text{L}^{-1}$)	Contact time (min)	Predicted C_0 ($\text{mg}\cdot\text{L}^{-1}$)	Microbial limit (CFU/100 mL)	Predicted CT ($\text{mg}\cdot\text{min}\cdot\text{L}^{-1}$)	Contact time (min)	Predicted C_0 ($\text{mg}\cdot\text{L}^{-1}$)
High mixing $\bar{G} = 18,158$ (s^{-1})	10^3	0.01	0.5	0.25	10^3	0.01	0.5	0.25
	10^2	0.1	0.5	0.43	10^2	0.08	0.5	0.39
	10^1	0.82	0.5	1.88	10^1	0.93	0.5	2.10
Low mixing $\bar{G} = 762$ (s^{-1})	10^3	0.5	60	0.47	10^3	0.45	60	0.46
	10^2	5.9	60	1.20	10^2	3.9	60	0.93
	10^1	48.5	60	7.01	10^1	47.5	60	6.88

Abbreviation: CFU, colony-forming units.

between injection and sampling as shown in Figure 2). The initial microbial concentration was assumed to be 10^4 CFU/100 mL, in accordance with experimental measurements. Table 3. presents predicted CTs and initial NaClO concentrations required to achieve specific limits for both total and fecal coliform.

Results demonstrate that application of a high mixing, pressured regime can significantly reduce the required CT. More specifically, for total coliforms, the CT to comply with regulations could be reduced by sixtyfold when high mixing is employed. This suggests a more efficient approach to achieving regulatory compliance, potential cost savings, less chemical use, and improved operational efficiency.

Additionally, given that use of sodium hypochlorite for wastewater disinfection can lead to formation of DBPs, a screening test for DBPs was conducted for the two mixing conditions. Specifically, the concentrations of several DBPs were evaluated with the experimental conditions and results presented in Table S12. Data reveal that, even at higher CT values, the concentration of DBPs remained low. Thus, it is possible to achieve effective microbial inactivation while controlling DBP formation.

Future work will entail a deeper investigation of the mechanism of the activation observed under high mixing, as well as confirming scale-up performance and energy costs by piloting the system (MITO₃X) at a higher flow-rate. Thus, based on pumping requirements, the associated energy demand per unit flow is anticipated to be between $0.06\text{--}0.11 \text{ kWh}\cdot\text{m}^{-3}$ to achieve effluent coliform concentrations of $10\text{--}100$ CFU/100 mL. With an average cost of electricity of $0.192 \text{ \$}\cdot\text{kW}^{-1}\cdot\text{h}^{-1}$, the electrical energy cost associated with this novel technology would be $\sim 0.007\text{--}0.021 \text{ \$}\cdot\text{m}^{-3}$, which is potentially competitive for the disinfection of wastewater with high tailing propensity such as granular sludge (GS) and biologically aerated filter (BAF) effluents.

CONCLUSIONS

Based on results of this investigation, following conclusions can be made:

- The impact of mixing intensity (quantified by velocity gradient) on municipal secondary wastewater disinfection by sodium hypochlorite was significant with high-mixing regimes requiring lower initial CT doses compared to low mixing.
- A coliform inactivation model incorporating the mean velocity gradient, $\bar{G}$, was proposed and assessed against batch and pilot data. Predictive modeling based on this proposed model indicated varying CT required to meet treatment objectives under different mixing conditions.
- Using the high-mixing technology tested in this study, efficient disinfection without tailing was achieved, and effluent coliform concentrations were as low as 1 CFU/100 mL at feasible CTs.
- DBP screening tests confirmed that enhanced inactivation under high-mixing regimes did not increase DBPs across all tested CT values.
- Future studies should focus on the scalability of the MITO₃X system and potential trade-offs between energy consumption and mixing efficiency in full-scale WWTPs. Additional research is needed to optimize the balance between energy use and disinfection performance, evaluate cost implications, and address challenges in large-scale implementation. These efforts will be essential for assessing the full feasibility of high-intensity mixing for wastewater treatment.

AUTHOR CONTRIBUTIONS

Naghmeh Fallah: Conceptualization; investigation; funding acquisition; writing – original draft; methodology; validation; visualization; writing – review and

editing; software; formal analysis; project administration; data curation. **Katherine Bell:** Writing – review and editing; conceptualization; visualization; resources. **Ted Mao:** Funding acquisition; resources. **Ronald Hofmann:** Conceptualization; investigation; data curation; resources; writing – review and editing; formal analysis. **Gabriela Ellen Barreto Bossoni:** Data curation. **Domenico Santoro:** Conceptualization; methodology; investigation; validation; funding acquisition; visualization; software; supervision; resources; project administration; writing – review and editing. **Giuseppe Mele:** Conceptualization; methodology; investigation; funding acquisition; validation; visualization; supervision; resources; writing – review and editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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