Published by
NIGERIAN SOCIETY OF PHYSICAL SCIENCES
Available online @ https://journal.nsps.org.ng/index.php/jnsps

J. Nig. Soc. Phys. Sci. 7 (2025) 3047

Journal of the Nigerian Society of Physical Sciences

Optimizing initial chlorine dosage at an injection point along a water distribution pipe

John Tulirinya[a,d,*], Mathew Kinyanju[b], Samuel Mutua[c], Asaph Muhumuza[d]

[a]*Department of Mathematics, Pan African University Institute for Basic Sciences, Technology and Innovation, Nairobi, 62000-00200, Kenya*
[b]*Department of Mathematics, Jomo Kenyatta University of Agriculture and Technology, Nairobi, 62000-00200, Kenya*
[c]*Department of Mathematics, Taita Taveta University, Voi, 635-80300, Kenya*
[d]*Department of Mathematics, Busitema University, Tororo, 236, Uganda*

Abstract

This study proposed a gradient-based optimization framework for determining the optimal initial chlorine dosage at an injection point along a water distribution pipe, with the aim of ensuring microbial safety and regulatory compliance while minimizing chlorine overuse and associated costs. Leveraging the SNOPT (Sparse Nonlinear Optimizer) algorithm integrated within the COMSOL Multiphysics environment, the approach systematically refined dosing strategies based on temperature-dependent chlorine decay dynamics. Prior to optimization, a uniform dosage of 1 mg/L yielded suboptimal outlet residuals; 0.30 mg/L, 0.23 mg/L, and 0.17 mg/L at 290K, 300K, and 310K, respectively. Post-optimization, precise dosing of 0.66 mg/L, 0.87 mg/L, and 1.16 mg/L achieved the target residual concentration of 0.2 mg/L across the same temperature conditions, enhancing disinfection control by 13-17%. The results demonstrate that this method delivers accurate, adaptive chlorine dosing, reducing the risk of harmful disinfection byproducts (DBPs), improving cost efficiency, and supporting sustainable water quality management. The proposed model is suitable for real-time integration into supervisory control systems, offering a practical pathway for advancing water safety, operational effectiveness, and environmental stewardship.

DOI:10.46481/jnsps.2025.3047

Keywords: Optimizing, Chlorine dosage, Chlorine residual, Water distribution pipe

Article History :
Received: 12 July 2025
Received in revised form: 12 August 2025
Accepted for publication: 15 August 2025
Available online: 22 September 2025

Communicated by: Oluwatobi Akande

1. Introduction

The provision of clean and safe drinking water remains a cornerstone of public health and sustainable development worldwide [1]. Across urban and rural contexts, water utilities are tasked with the complex challenge of maintaining water quality as it moves through extensive distribution networks [2]. Chlorination is the most widely employed method for disinfecting water due to its affordability and proven efficacy. However, maintaining effective residual chlorine concentrations throughout a distribution network is a nuanced endeavor [3]. Chlorine decays over time due to chemical reactions and environmental factors, such as temperature and flow dynamics, raising concerns of under-dosing, which compromises microbial safety, and overdosing, which leads to the formation of harmful disinfection byproducts (DBPs) [4].

Globally and regionally, water quality standards mandate

*Corresponding author Tel. No.: +25-670-321-4138.
Email address: tulirinyajohn@gmail.com (John Tulirinya)

minimum residual chlorine concentrations to safeguard against microbial contamination. For instance, the World Health Organization (WHO) recommends a minimum residual concentration of 0.2 mg/L for domestic water safety [5]. However, achieving this target consistently across spatially and temporally variable network conditions presents a persistent operational challenge. In many low and middle-income regions, including parts of Sub-Saharan Africa, the optimization of chlorine dosing remains limited by technical, computational, and economic constraints [6]. These challenges are further magnified in real-world networks with complex topologies and variable demand patterns.

Traditionally, water utilities have relied on trial-and-error methods or heuristic-based optimization techniques such as Genetic Algorithms (GA), Particle Swarm Optimization (PSO), and Bayesian Optimization (BO) [7]. While these methods have shown promise, they often suffer from high computational costs, slow convergence, and limitations in handling high-dimensional constraints, especially those governed by nonlinear partial differential equations (PDEs). These limitations point to a significant gap in the availability of fast, accurate, and scalable optimization strategies that can be deployed in operational environments. In response to this gap, the present study explored a gradient-based optimization framework to determine the optimal initial chlorine dosage at an injection point along a water distribution pipe. Using the SNOPT (Sparse Nonlinear OPTimizer) solver integrated within COMSOL Multiphysics, the study aims to minimize deviations from a target chlorine residual concentration at the network outlet. This approach leverages local derivative information for more efficient convergence while satisfying physical and regulatory constraints on chlorine transport and decay.

The scope of this study was confined to optimizing the initial chlorine concentration at a single injection point under varying temperature conditions. While the model does not yet account for seasonal fluctuations, variable demand, or multi-point injections, it serves as a foundational step toward real-time, model-based chlorine management systems. The optimization process is evaluated under different thermal conditions to assess its robustness and responsiveness to environmental variations.

By enhancing chlorine residual control through this model-based optimization, the study contributes to improved microbial safety, regulatory compliance, and cost efficiency. The methodology proposed holds promise for integration into supervisory control and data acquisition (SCADA) systems, enabling dynamic and automated chlorine dosing in response to real-time network conditions. This contributes not only to operational excellence but also to public health protection and environmental sustainability by minimizing chlorine wastage and DBP formation.[7]

2. Literature review

The study by Ref. [8] compared Bayesian Optimization (BO) with Evolutionary Algorithms (EAs), specifically Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), for optimizing chlorine dosage in water distribution systems (WDSs) using a multi-species water quality (MS-WQ) model. Traditional EAs require many computationally expensive simulations, making them less efficient for large-scale WDSs. The study evaluated these methods using a real-life WDS case study and found that BO is significantly more efficient, requiring fewer function evaluations and exhibiting faster convergence while maintaining high accuracy.

According to Ref. [9], the optimization of the ozonation process in drinking water treatment to minimize disinfection by-products (DBPs) while ensuring safe water quality was explored. Using a Box–Behnken experimental design, the study modeled the effects of ozone dose and treatment duration on the formation of bromate. Two treatment strategies were tested: Strategy 1, which aimed to minimize all DBPs, and Strategy 2, which focused on controlling bromate formation while keeping other DBPs below 80% of regulatory limits. The findings indicated that Strategy 2 is more cost-effective, reducing ozone consumption while maintaining water quality within legal standards.

In the study of Ref. [10], the breadth-first search (BFS) algorithm and genetic algorithm (GA) were applied to optimize chlorine dosage injection in water distribution networks to maintain spatial and temporal residual chlorine levels within an acceptable range. This chlorine dosage injection estimation was based on water age to maintain a minimum of 0.2 mg/L residual chlorine at demand nodes. Results indicated that the water age-based chlorine estimation has an average error below 10%, and a four-interval injection scheme is effective in adapting to demand fluctuations.

Although, numerous numerical optimization techniques have been explored for chlorine dosage optimization in water distribution networks (WDNs), each with its strengths and limitations. Evolutionary Algorithms, such as Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), are broadly used due to their ability to handle nonlinear and complex objective functions [11]. However, they necessitate extensive function evaluations, making them computationally expensive, especially for large-scale networks [12]. Bayesian Optimization (BO) is being proposed as a more efficient alternative, as it reduces the number of function evaluations by using probabilistic surrogate models [13]. Nonetheless, it still struggles with handling high-dimensional problems and nonlinear PDE constraints [14], limiting its effectiveness in detailed chlorine transport modeling. Derivative-free solvers, such as Coordinate Search and Nelder-Mead, avoid gradient computation but often converge slowly and may get trapped in local optima [15]. This study introduces a gradient-based optimization approach using SNOPT within COMSOL Multiphysics, which achieves faster convergence with fewer function evaluations [16]. By doing so, it provides a more efficient and scalable solution for real-time chlorine dosage optimization, enhancing microbial safety, regulatory compliance, and operational cost-effectiveness.

This present study has significant practical implications for water utility companies and regulatory agencies responsible for ensuring safe and clean water. By optimizing the initial chlorine dosage, the required chlorine residual levels are maintained throughout the distribution network. This ensures microbial

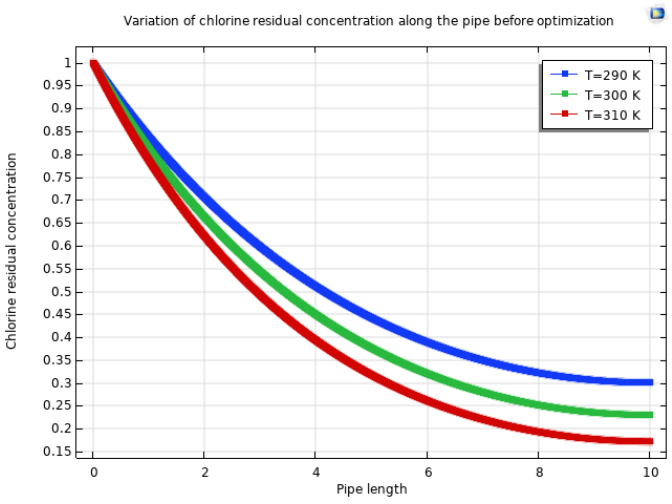

Figure 1. Chlorine residual concentration profile along the pipeline at three temperatures (290K, 300K, 310K) before optimization.

safety compliance with regulatory standards while reducing operational costs associated with over-chlorination. Ultimately, this optimization strategy enhances public health protection, cost efficiency, and environmental sustainability in water treatment and distribution.

3. Optimization model

3.1. Parameter optimization with COMSOL multiphysics

Parameter optimization involves finding values for a model parameter to meet certain constraint(s) such that an optimal value for a particular parameter is obtained. Parameter optimization with COMSOL Multiphysics mainly involves four sections namely; selecting an appropriate optimization solver, developing objective function, defining control variables and parameters, as well as the constraints to which the objective function is subjected.

The objective function minimized in this study is the total deviation of the chlorine residual concentration level at point along the water distribution network from the acceptable/target chlorine concentration. The constraints are; chlorine residual concentration limits and initial chlorine concentration dosage at the pipe inlet. Table 1 shows a list of variables and parameters that were utilized in the study.

3.2. Objective function

To optimize initial chlorine concentration dosage at the injection point such that the desired/target chlorine residual concentration at any pipe outlet over time is maintained while avoiding under and overdosing.

$$Min\ J(c_0) = \frac{1}{2}\sum_{t=1}^{T}\left(C(c_0,t) - C_T\right)^2, \tag{1}$$

where J is the total deviation from the desired chlorine residual concentration, $C(c_0,t)$ is the chlorine residual concentration at the pipe outlet at time t, C_T is the target/desired chlorine residual concentration at the pipe outlet.

3.3. Constraints of the objective function

The objective function is subject to the following constraints:

3.3.1. Chlorine residual transport

The chlorine residual concentration is computed from [21]:

$$\frac{\partial C}{\partial t} + u_z\frac{\partial C}{\partial z} = \frac{1}{Pe}\left(\frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2} + \frac{\partial^2 C}{\partial z^2}\right) - \left(Da + \beta_1 e^{-E/RT}\right)C. \tag{2}$$

where Peclet number $Pe = \frac{LU}{D}$, Damköhler number: $Da = \frac{Lk_1}{U}$, and $\beta_1 = \frac{LA}{U}$, L and U are characteristic length and velocity respectively, C is the concentration of chlorine residual at time t, D is the molecular diffusivity, k_1 total decay chlorine reaction rate (due to both bulk and wall decay rates), A is Arrhenius or frequency factor, E is Arrhenius activation energy, T is temperature, and R is ideal gas constant.

Initial and boundary conditions

i. At $t = 0$, $C = 1$, $z \geq 0$.
ii. symmetric condition ($r = 0$); $\frac{\partial C}{\partial r} = 0$.
iii. at the pipe wall ($r = R$); No flux,($\frac{\partial C}{\partial r} = 0$).
iv. at the inlet; $C = 1$, $t \geq 0$.
v. at the outlet ($z = L$); $\frac{\partial C}{\partial z} = 0$.

3.3.2. Chlorine residual concentration limits

Chlorine residual concentration levels must remain within permissible bounds.

$$C_{min} \leq C \leq C_{max}, \tag{3}$$

where $C_{min} = 0.2\ mg/L$ and $C_{max} = 0.5\ mg/L$ are the minimum and maximum chlorine residual concentration levels respectively, permissible for safe water to be consumed domestically [17].

3.4. Control parameter

The initial chlorine dosage concentration, c_0 at the injection point/pipe inlet was considered as the control parameter for this study.

$$0 \leq c_0 \leq m, \tag{4}$$

where m is the upper limit of possible chlorine dosage, with $m = 5$ by WHO [18]. If $c_0 = 0$, then no chlorine is dosed at injection/inlet point.

3.5. Optimization solver

The Optimization Module in COMSOL Multiphysics software offers a variety of optimization solver algorithms, categorized into two primary types: gradient-based solvers and derivative-free solvers as described in [19]. These categories are tailored to address distinct problem scenarios and exhibit differing performance attributes.

Table 1. List of variables and parameters

Symbol	Description	Unit
C	Chlorine residual concentration at time t	mg/L
C_T	Target chlorine residual concentration at the outlet	mg/L
c_0	Initial chlorine dosage concentration at the injection point	mg/L
t	Time	s
z	Axial coordinate along the pipe	m
r	Radial coordinate in the pipe cross-section	m
D	Molecular diffusivity of chlorine in water	m^2/s
u_z	Flow velocity along the pipe	m/s
Pe	Péclet number ($Pe = LU/D$)	Dimensionless
Da	Damköhler number ($Da = Lk_1/U$)	Dimensionless
k_1	Total chlorine decay reaction rate	s^{-1}
β_1	Arrhenius factor	Dimensionless
E	Arrhenius activation energy	J/mol
T	Temperature of the water	K
R	Ideal gas constant	J/(mol·K)
$J(c_0)$	Objective function representing total deviation from target chlorine residual concentration	-
M	Mass matrix in the finite element discretization	-
A	Stiffness and advection matrix in the finite element discretization	-

3.5.1. Gradient-based solvers

Gradient-based solvers are basically utilized in cases where each new iterate is based on local derivative information evaluated at previously visited points. The different gradient-based algorithms include; SNOPT and IPOPT solvers which handle large-scale problems with numerous or hard constraints, MMA solver which best handles problems with a huge number of control variables, and Levenberg–Marquardt solver which explicitly solves least-squares problems.

3.5.2. Derivative-free solvers

With derivative-free solvers, there is no need to compute any derivative of the objective function with respect to the control variables. The four different derivative-free algorithms in COMSOL Multiphysics include; Coordinate search solver which targets at improving the objective function along the coordinate directions of the control variable space, Nelder–Mead solver which aims at improving the objective function values by iteratively replacing the worst corner of a simplex in the control variable space, BOBYQA solver which aims at improving the objective function values by using an iteratively constructed quadratic approximation of the objective, and COBYLA solver which solves a sequence of linear approximations constructed from objective and constraint values sampled at the corners of a simplex in control variable space.

In this study, SNOPT which is a gradient-based solver was utilized due to its computational efficiency in handling nonlinear PDE constraint optimization problems.

4. Method of solution

Finite Element Method (FEM) was utilized to solve the chlorine residual transport equation (2) with COMSOL Multiphysics. Below is the FEM discretization process;

4.1. Weak formulation

Multiplying equation (2) by a test function $\phi(r, z)$ and integrating over the domain Ω yields:

$$\int_\Omega \left(\frac{\partial C}{\partial t} + u_z \frac{\partial C}{\partial z} - \frac{1}{Pe} \left(\frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2} + \frac{\partial^2 C}{\partial z^2} \right) \right) \phi d\Omega + \int_\Omega \left(\left(Da + \beta_1 e^{-E/RT} \right) C \right) \phi d\Omega = 0. \tag{5}$$

Applying integration by parts to the diffusion terms and considering the given boundary conditions:

$$\int_\Omega \frac{\partial C}{\partial t} \phi d\Omega + \int_\Omega u_z \frac{\partial C}{\partial z} \phi d\Omega + \frac{1}{Pe} \int_\Omega \frac{\partial \phi}{\partial r} \frac{\partial C}{\partial r} d\Omega + \frac{1}{Pe} \int_\Omega \frac{\partial \phi}{\partial z} \frac{\partial C}{\partial z} d\Omega + \int_\Omega \left(Da + \beta_1 e^{-E/RT} \right) C \phi d\Omega = 0. \tag{6}$$

4.2. Finite element discretization

Approximating the concentration field $C(r, z, t)$ using finite element shape functions:

$$C(r, z, t) \approx \sum_{j=1}^{N} C_j(t) \psi_j(r, z), \tag{7}$$

where $\psi_j(r, z)$ are the basis functions and $C_j(t)$ are the unknown nodal values.

Similarly, we choose the test function $\phi(r,z) = \psi_i(r,z)$, leading to the system:

$$\sum_{j=1}^{N}\left[\int_\Omega \phi_i\psi_j d\Omega\right]\frac{dC_j}{dt} + \sum_{j=1}^{N}\left[\int_\Omega \phi_i u_z \frac{\partial\psi_j}{\partial z} d\Omega\right]C_j + \frac{1}{Pe}\sum_{j=1}^{N}\left[\int_\Omega\left(\frac{\partial\phi_i}{\partial r}\frac{\partial\psi_j}{\partial r} + \frac{\partial\phi_i}{\partial z}\frac{\partial\psi_j}{\partial z}\right)d\Omega\right]C_j + \sum_{j=1}^{N}\left[\int_\Omega \phi_i\left(Da + \beta_1 e^{-E/RT}\right)\psi_j d\Omega\right]C_j = 0. \quad (8)$$

This equation can be written in matrix form:

$$M\frac{dC}{dt} + AC = 0, \quad (9)$$

where M is the mass matrix: $M_{ij} = \int_\Omega \phi_i\psi_j d\Omega$ and A is the stiffness and advection matrix:

$$A_{ij} = \int_\Omega \phi_i u_z \frac{\partial\psi_j}{\partial z} d\Omega + \frac{1}{Pe}\int_\Omega\left(\frac{\partial\phi_i}{\partial r}\frac{\partial\psi_j}{\partial r} + \frac{\partial\phi_i}{\partial z}\frac{\partial\psi_j}{\partial z}\right)d\Omega + \int_\Omega \phi_i\left(Da + \beta_1 e^{-E/RT}\right)\psi_j d\Omega. \quad (10)$$

4.3. Time discretization

The implicit Euler method was utilized for time-stepping;

$$M\frac{C^{n+1} - C^n}{\Delta t} + AC^{n+1} = 0. \quad (11)$$

Rearranging for C^{n+1} yields:

$$(M + A\Delta t)C^{n+1} = MC^n. \quad (12)$$

System (11) was finally solved at each time step using a COMSOL Multiphysics software.

4.4. Reformulating the optimization problem for SNOPT

SNOPT is based on Sequential Quadratic Programming (SQP), a powerful method for solving constrained nonlinear optimization problems. SNOPT solves problems in a standard optimization form [20];

$$\min f(x). \quad (13)$$

subject to:

$$g(x) = 0,$$
$$h_0 \le h(x) \le h_u,$$
$$x_0 \le x \le x_u,$$

where $x = c_0$ is the decision variable, $f(x) = J(c_0)$ is the objective function, $g(x)$ and $h(x)$ represents the equality and inequality constraints respectively, l_0 and x_0 are lower constraint bounds and l_u and x_u are upper constraint bounds.

4.4.1. Defining $g(x)$ and $h(x)$

The constraint function $g(x)$ is given as;

$$g(x) = M\frac{dC}{dt} + AC = 0, \quad (14)$$

and the constraint function $h(x) = \begin{bmatrix} C \\ c_0 \end{bmatrix}$, is defined as;

$$\begin{bmatrix} 0.2 \\ 0 \end{bmatrix} \le \begin{bmatrix} C \\ c_0 \end{bmatrix} \le \begin{bmatrix} 0.5 \\ 5 \end{bmatrix}. \quad (15)$$

4.5. SQP subproblem formulation

Sequential Quadratic Programming (SQP) solves nonlinear optimization problems iteratively by approximating the problem with a quadratic programming (QP) subproblem at each iteration, k.

4.5.1. Lagrangian function

At each iteration k, a quadratic model of the Lagrangian is formed. The Lagrangian function combines the objective function and the constraints into a single scalar-valued function. The Lagrangian function of our problem is defined as;

$$\mathcal{L}(c_0, \lambda, \mu) = J(c_0) - \lambda^T g(c_0) - \mu^T h(c_0), \quad (16)$$

where λ is the Lagrange multiplier vector for equality constraint and μ is the Lagrange multiplier vector for inequality constraints. The Hessian matrix of the Lagrangian function is then given by:

$$H = \nabla^2\mathcal{L}(c_0, \lambda, \mu). \quad (17)$$

The Karush-Kuhn-Tucker (KKT) conditions below, help to determine the Lagrange multipliers:

i. Stationarity condition: The gradient of the Lagrangian must be zero at the optimal solution.

$$\nabla L(c_0, \lambda, \mu) = \nabla J(c_0) - \nabla g(c_0)^T\lambda - \nabla h(c_0)^T\mu = 0. \quad (18)$$

ii. Primal feasibility condition: The solution must satisfy the original constraints.

$$g(c_0) = 0, \quad h_0 \le h(c_0) \le h_u. \quad (19)$$

iii. Dual feasibility condition: For inequality constraints, the multipliers must be non-negative.

$$\mu_j \ge 0, \quad \forall j. \quad (20)$$

iv. Complementary slackness condition. For each inequality constraint, either the constraint is active (binding) or its multiplier is zero.

$$\mu_j \cdot (h_j(c_0) - h_{0,j}) = 0, \quad \mu_j \cdot (h_{u,j} - h_j(c_0)) = 0. \quad (21)$$

This ensures that if a constraint is strictly within bounds, its multiplier is zero; otherwise, the multiplier is positive.

4.5.2. Linearizing the KKT system

To construct a Quadratic Programming (QP) subproblem in Sequential Quadratic Programming (SQP), we linearize the constraints and stationarity condition using a first-order Taylor expansion.

Stationarity Condition:

The stationarity condition of the optimization problem states that at an optimal point, the gradient of the Lagrangian function must be zero.

$$\nabla J(c_0) - \nabla g(c_0)^T \lambda - \nabla h(c_0)^T \mu = 0. \tag{22}$$

For the objective function, we approximate the gradient of the objective function $J(c_0)$ near the current iterate c_0 as follows:

$$\nabla J(c_0 + d) \approx \nabla J(c_0) + \nabla^2 J(c_0) d. \tag{23}$$

For the constraint functions, we linearize the constraint functions themselves, not their gradients.

For the equality constraints:

$$g(c_0 + d) \approx g(c_0) + \nabla g(c_0) d. \tag{24}$$

For the inequality constraints:

$$h(c_0 + d) \approx h(c_0) + \nabla h(c_0) d. \tag{25}$$

For the stationarity condition:

$$\nabla L(c_0 + d, \lambda, \mu) \approx \nabla L(c_0, \lambda, \mu) + \nabla^2 L(c_0, \lambda, \mu) d = 0. \tag{26}$$

$$\implies \nabla L(c_0, \lambda, \mu) = -\nabla^2 L(c_0, \lambda, \mu) d. \tag{27}$$

Equation (27) becomes;

$$\nabla J(c_0) - \nabla g(c_0)^T \lambda - \nabla h(c_0)^T \mu = -\nabla^2 L(c_0, \lambda, \mu) d. \tag{28}$$

But $\nabla^2 L(c_0, \lambda, \mu) = \nabla^2 J(c_0)$.

Equation (28) becomes;

$$\nabla J(c_0) - \nabla g(c_0)^T \lambda - \nabla h(c_0)^T \mu = -\nabla^2 J(c_0) d. \tag{29}$$

Rearranging equation (29), we obtain:

$$\nabla^2 J(c_0) d - \nabla g(c_0)^T \lambda - \nabla h(c_0)^T \mu = -\nabla J(c_0). \tag{30}$$

These linearizations are used to construct the QP subproblem. Solving this QP yields a search direction d, which is used to update the current iterate c_0, typically via a line search:

$$c_1 = c_0 + \alpha d, \tag{31}$$

where $\alpha \in (0, 1]$ is a step size chosen to ensure sufficient decrease and constraint feasibility.

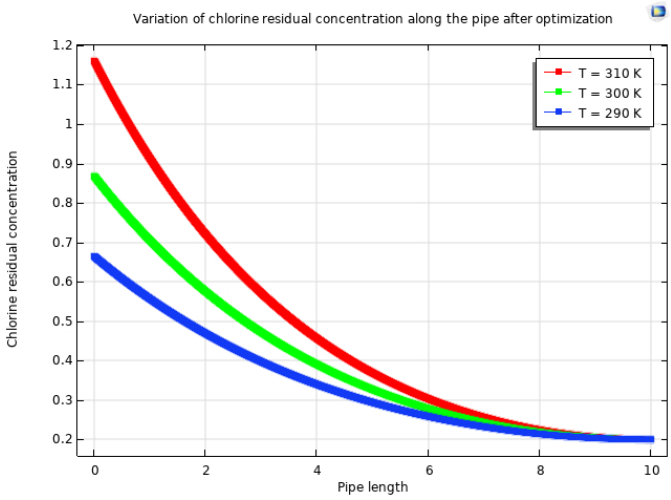

Figure 2. Optimized chlorine residual concentration profiles at 290K, 300K, and 310K.

4.6. Matrix form of the linearized system

The linearized stationarity condition is incorporated into the full Sequential Quadratic Programming (SQP) subproblem:

$$\begin{bmatrix} \nabla^2 J & -\nabla g^T & -\nabla h^T \\ \nabla g & 0 & 0 \\ \nabla h & 0 & D \end{bmatrix} \begin{bmatrix} d \\ \lambda \\ \mu \end{bmatrix} = \begin{bmatrix} -\nabla J \\ 0 \\ 0 \end{bmatrix}, \tag{32}$$

where $\nabla^2 J$ is the Hessian of the objective function, ∇g is the Jacobian matrix of the equality constraints, ∇h is the Jacobian matrix of the inequality constraints, D ensures $\mu \geq 0$, for handling inequality constraints.

This system is solved iteratively within the SQP algorithm to update the decision variable c_0 and the Lagrange multipliers λ and μ.

At each iteration k, the Sequential Quadratic Programming (SQP) method solves the following Quadratic Programming (QP) subproblem:

$$\min_d \quad \frac{1}{2} d^T H_k d + \nabla J(c_0^k)^T d. \tag{33}$$

subject to:

$$\nabla g(c_0^k) d + g(c_0^k) = 0. \tag{34}$$

$$h_0 - h(c_0^k) \leq \nabla h(c_0^k) d \leq h_u - h(c_0^k), \tag{35}$$

where d is the search direction (step from the current iterate c_0^k), H_k is the Hessian approximation of the Lagrangian function at c_0^k, $\nabla J(c_0^k)$ is the gradient of the objective function at c_0^k, $\nabla g(c_0^k)$ and $\nabla h(c_0^k)$ are the Jacobian matrices of the equality and inequality constraints, respectively.

4.7. SNOPT Algorithm Implementation

Algorithm 1 SNOPT Algorithm Implementation

1: Initialize c_0
2: Solve the PDE using FEM to obtain $C(c_0, t)$
3: Compute the objective function $J(c_0)$
4: Evaluate the gradient $\nabla J(c_0)$
5: Solve the SQP subproblem to find new c_0
6: Update c_0 and iterate until convergence

5. Results and discussion

Figure 1 illustrates the variation of chlorine residual concentration along the length of a pipe at three temperatures (290 K, 300 K, and 310 K) before optimization. In all cases, there is a clear monotonic decline in chlorine residual concentration with increasing pipe length. This pattern reflects the combined effects of chlorine decay processes such as bulk-phase reactions with natural organic matter, reactions with inorganic species, and potential catalytic effects from the pipe wall material. Additionally, transport phenomena such as advection and dispersion contribute to the observed decrease.

The differences between the curves highlight the strong influence of temperature on chlorine stability. At higher temperatures (310 K), chlorine decays more rapidly, producing a steeper slope. This is likely due to the temperature dependence of reaction kinetics, as elevated temperatures typically accelerate chemical reaction rates according to the Arrhenius equation. Conversely, at lower temperatures (290 K), reaction rates slow down, preserving higher chlorine residuals over longer distances.

These results carry practical implications for water distribution systems. In warmer climates or during summer months, chlorine concentrations may drop below required thresholds before reaching the far ends of the network, potentially compromising microbial safety. In contrast, cooler conditions extend chlorine persistence, allowing for more stable disinfection but potentially increasing the formation of disinfection byproducts if the residual remains high for prolonged periods. Therefore, understanding the interplay between temperature and chlorine decay is essential for designing dosing strategies, selecting pipe materials, and planning operational adjustments to maintain safe and compliant water quality at all points in the network.

Figure 2 depicts the variation of chlorine residual concentration along the pipe length for three operating temperatures: 310 K, 300 K, and 290 K after the application of an optimization process. The curves maintain the characteristic exponential decay pattern, confirming that chlorine concentration continues to diminish as water moves through the pipe due to ongoing bulk and wall reactions, as well as transport-related losses. However, compared to the pre-optimization scenario, the initial chlorine concentrations are noticeably higher, reflecting the adjustment made at the injection point to meet residual targets at the far end of the distribution segment.

The results indicate that higher operating temperatures necessitate a greater initial chlorine dose to counteract the more rapid decay rates driven by increased reaction kinetics. This is evident from the 310 K curve, which starts at the highest concentration yet still declines more steeply than the lower temperature curves. Conversely, at 290 K, decay rates are slower, and the initial dosage requirement is correspondingly smaller.

The optimization objective of balancing microbial safety with minimization of excessive chlorine loss appears to have been achieved. In all three temperature scenarios, the terminal chlorine concentration converges to a similar acceptable threshold, ensuring regulatory compliance and public health protection while avoiding unnecessarily high residuals that could contribute to disinfection byproduct formation or customer complaints about taste and odor.

These findings highlight the operational value of adaptive chlorine dosing strategies in water distribution systems. By incorporating temperature-dependent decay characteristics into the optimization model, utilities can dynamically adjust injection dosages seasonally or in response to temperature fluctuations, thereby enhancing both water quality and system efficiency. The post-optimization profiles also demonstrated that targeted interventions can mitigate the risks associated with variable decay rates without over-reliance on conservative overdosing practices.

6. Conclusion

The optimization process improved chlorine retention, as indicated by the chlorine residual concentration at the outlet not going below the target of 0.2 as recommended by WHO. Interestingly, the ordering of concentration trends remains the same (higher temperature leads to lower concentration retention), but the overall concentrations are significantly improved. This suggests that the optimization has enhanced chlorine persistence, likely improving disinfection efficiency throughout the water distribution pipe.

While the optimization framework demonstrated strong performance within the COMSOL Multiphysics simulation environment, the present study did not directly validate the results in a real-world water distribution system. This work was intended as a foundational modeling and optimization step, providing the necessary computational insights before field implementation. Future research will focus on practical deployment and experimental validation in operational water distribution networks, where the optimized dosing strategy will be tested under real hydraulic, environmental, and demand conditions. Such validation will be essential to confirm the framework's robustness and effectiveness when subject to the uncertainties and complexities inherent in real-world systems.

Data availability

No additional data was used beyond those presented in the submitted manuscript.

Acknowledgment

The authors thank the African Union through the Pan African University Institute for Basic Sciences, Technology, and Innovation for the financial support that made this work possible.

References

[1] C. O. Okafor, U. I. Ude, F. N. Okoh & B. O. Eromonsele, *Safe drinking water: the need and challenges in developing countries*, in *Water quality - new perspectives*, I. Sarbu and S. Popa-Albu (Eds.), IntechOpen, London, UK, 2024, pp. 144–155. https://doi.org/10.5772/intechopen.108497.

[2] M. E. Machweu, *Addressing high dimensionality in water quality modelling in water distribution networks*, M.Sc. dissertation, University of the Witwatersrand, Johannesburg, South Africa, 2024. https://wiredspace.wits.ac.za/server/api/core/bitstreams/16e66b06-4dd8-4dab-9c09-1625279d0193/content.

[3] S. Yan, P. Drogui, R. D. Tyagi & J. W. C. Wong, *Development of decentralized drinking water treatment plant*, in *Decentralized sanitation and water treatment: concept and technologies*, London, UK, 2024, pp. 139–153. https://doi.org/10.1201/9781003381419-11.

[4] A. Gani, M. Singh, S. Patha & A. Hussain, *Recent advancements in chlorine applications for water quality control*, in *Drinking water disinfection by-products: sources, fate and remediation*, Springer nature, London, UK, pp. 35–58. https://doi.org/10.1007/978-3-031-49047-7_3.

[5] I. Hespanhol & A. Prost, "WHO guidelines and national standards for reuse and water quality", Water Research **28** (1994) 119. https://www.sciencedirect.com/science/article/pii/0043135494901252

[6] B. Gael Fouda-Mbanga, T. Seyisi, Y. Boitumelo Nthwane, B. Nyoni & Z. Tywabi-Ngeva, "A review on pollutants found in drinking water in Sub-Sahara African rural communities: detection and potential low-cost remediation methods", Industrial and Domestic Waste Management **3** (2023) 67. https://doi.org/10.53623/idwm.v3i2.264

[7] I. Sarbu & S. Popa-Albu, "Optimization of urban water distribution networks using heuristic methods: an overview", Water International **48** (2023) 120. https://doi.org/10.1080/02508060.2022.2127611.

[8] M. Moeini & A. Abokifa, "Chlorine dosage management in drinking water systems: comparing Bayesian optimization to evolutionary algorithms", Journal of Hydroinformatics **26** (2024) 2720. https://doi.org/10.2166/HYDRO.2024.090.

[9] M. Gregov, J. G. Kljusurić, D. Valinger, M. Benković, T. Jurina, A. J. Tušek, V. Crnek, M Matošić, "Optimization of Ozonation in drinking water production at Lake Butoniga", Water **17** (2025) 97. https://doi.org/10.3390/W17010097/S1.

[10] F. D. Frederick, M. S. Marlim & D. Kang, "Optimization of chlorine injection schedule in water distribution networks using water age and breadth-first search algorithm, Water **16** (2024) 486. https://doi.org/10.3390/W16030486.

[11] N. T. Linh, "A novel combination of genetic algorithm, particle swarm optimization, and teaching-learning-based optimization for distribution network reconfiguration in case of faults", Engineering, Technology & Applied Science Research **14** (2024) 12959. https://doi.org/10.48084/ETASR.6718.

[12] X. Song, Y. Zhang, W. Zhang, C. He, Y. Hu, J. Wang & D. Gong, "Evolutionary computation for feature selection in classification: a comprehensive survey of solutions, applications and challenges", Swarm and Evolutionary Computation **90** (2024) 101661. https://doi.org/10.1016/J.SWEVO.2024.101661.

[13] R. Naveiro and B. Tang, "Simulation based Bayesian optimization", 2024. [Online]. https://arxiv.org/abs/2401.10811.

[14] H. F. Maathuis, R. De Breuker & S. G. P. Castro, "High-dimensional Bayesian optimisation with large-scale constraints via latent space Gaussian processes", 2024. [Online]. https://arxiv.org/abs/2412.15679.

[15] J. Zeijden "A hybrid method for numerical optimization", 2025.[Online]. https://fse.studenttheses.ub.rug.nl/id/eprint/34694.

[16] A. J. Joshy and J. T. Hwang, "Modopt: a modular development environment and library for optimization algorithms", 2024. [Online]. https://arxiv.org/abs/2410.12942.

[17] E. Zerrouk, "How WASH supports social justice in a changing climate: the importance of Water", Revista Tecnológica - ESPOL **37** (2025) 121. https://doi.org/10.37815/RTE.V37N1.1274.

[18] World Health Organization, "Nickel in drinking water: background document for development of WHO Guidelines for drinking-water quality", 2021. [Online]. https://iris.who.int/handle/10665/350934.

[19] T. Slawig, U. Prüfert & ZIK Virtuhcon, "Mathematics-based optimization in the COMSOL Multiphysics framework", COMSOL Conference, Stuttgart, Germany, 2011, pp. 110–116. https://www.comsol.jp/paper/download/83389/slawig_paper.pdf.

[20] E. Philip, W. Murray & M. A. Saunders, "User's guide for SNOPT version 7: software for large-scale nonlinear programming", UCSD, San Diego, CA, USA, 2019, pp. 15–21. https://ccom.ucsd.edu/reports/UCSD-CCoM-19-01.pdf.

[21] J. Tulirinya, M. Kinyanjui, S. Mutua & A. Muhumuza, "A two-dimensional mathematical model of chlorine residual transport in a water distribution pipe", Engineering Reports **7** (2025) e70325. https://doi.org/10.1002/eng2.7032510.1002/eng2.70325.