DeePC Based Strategy for the IJCAI-2025 Drinking Water Chlorination Challenge

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Abstract

This work introduces a data-driven predictive control strategy tailored for the *1st AI for Drinking Water Chlorination Challenge @ IJCAI-2025*. The approach employs a Data-Enabled Predictive Control (*DeePC*) paradigm, which reconstructs system dynamics from historical input–output trajectories encoded via Hankel matrices. By formulating a constrained quadratic program in the null-space of past measurements, the controller anticipates future chlorination demands and computes actuator trajectories that minimize disinfectant usage, ensure compliance with regulatory thresholds, and mitigate infection risk during contamination events. The design integrates actuator and sensor constraints explicitly, accommodates slack for feasibility under uncertainty, and reuses optimized plans to reduce computational overhead. Empirical evaluations across several scenarios reveal that the proposed controller achieves a balanced trade-off between operational cost, water quality assurance, and spatial fairness. This contribution exemplifies the potential of model-free, optimization-based control for enhancing resilience and safety in intelligent water distribution systems.

1 Introduction

Access to clean and safe drinking water remains a critical global imperative, with over two billion people currently relying on contaminated sources. To ensure microbiological safety, chlorination is widely used as a primary disinfection strategy. When appropriately dosed, chlorine inactivates pathogenic microorganisms and provides a residual disinfectant barrier throughout the distribution system. However, both under- and over-dosing can have severe consequences: insufficient chlorine may lead to pathogen survival or regrowth, while excessive dosing can result in toxic disinfection by-products and pipe corrosion. Maintaining appropriate chlorine levels is particularly challenging in real-world water distribution systems, which exhibit high-dimensional dynamics due to fluctuating demand, varying travel times, and limited sensor coverage. Moreover, chlorine decay is nonlinear and influenced by water temperature, age, organic matter, and pipe wall reactions. As such, the development of intelligent, adaptive chlorination control strategies that optimize disinfection efficacy while minimizing chemical usage and ensuring safety is an ongoing research challenge.

1.1 Competition Problem Statement

The **1st AI for Drinking Water Chlorination Challenge @ IJCAI-2025**, organized by the *ERC-WaterFutures* project team, presents a realistic and high-fidelity simulation benchmark to address this challenge. Participants are tasked with controlling chlorine injection at five designated chlorine boosters in a medium-scale water distribution network over a simulated 365-day period. The simulator is based on EPANET-MSX and accessed via the EPyT-Control interface [Vrachimis *et al.*, 2024].

Control decisions must be made based solely on sparse, real-time observations from 19 strategically placed sensors, comprising 2 flow meters and 17 chlorine concentration sensors. The environment features stochastic contamination events, uncertain water demand profiles, and nonlinear quality transport processes.

The evaluation of submitted controllers is based on the following key metrics:

- Total chlorine usage,
- Bounds violations,
- Bounds violations fairness,
- Injections smoothness,
- Infection risk

The full description of these objectives can be found in the competition repository[1]. The challenge is to develop robust, data-driven AI controllers that generalize across uncertainty, react to unforeseen contamination, and operate under partial observability. The approach presented in this work exemplifies such a solution through a principled optimization framework based on Data-Enabled Predictive Control (DeePC) @[Coulson *et al.*, 2019].

[1]https://github.com/WaterFutures/AI-for-Drinking-Water-Chlorination-Challenge-IJCAI-25

1.2 Challenges and Contributions

Managing chlorine injection in dynamic networks requires balancing multiple, often conflicting, objectives. The controller must minimize disinfectant usage while ensuring that residual concentrations comply with safety regulations and remain sufficiently robust to counteract contamination. These trade-offs are exacerbated by practical limitations, including actuator saturation, sparse sensor placement, demand uncertainty, and the nonlinear, time-varying decay of chlorine. Additionally, the propagation of contaminants and disinfectants depends on uncertain flow dynamics, further complicating real-time decision-making.

Traditional control methods, such as model predictive control (MPC), typically rely on accurate system models. However, such approach face a strict computational due to physical systems modeling involving nonlinear equations. Moreover, in data-scarce or highly uncertain environments, these approaches can fail to generalize or maintain feasibility. In contrast, emerging AI-based strategies, including reinforcement learning and data-driven optimization, offer a compelling alternative by learning behavior from past data and adapting to system evolution without requiring explicit physical models.

We propose a novel Data-Enabled Predictive Control (DeePC) framework tailored to the competition environment. Our main contributions are as follows:

- A DeePC-based controller that leverages historical trajectories to compute feasible, optimized chlorine injection plans.
- A quadratic programming formulation that jointly minimizes chemical cost, constraint violations, and infection risk.
- A hybrid control architecture combining DeePC with a fallback PID policy to ensure resilience and safety.
- Empirical validation of robustness and generalization across multi-scenario environments specified in the competition.

2 Methodology

This section details the mathematical formulation and implementation of the proposed **Data-Enabled Predictive Control (DeePC)** framework, developed for real-time optimization of chlorine injection in drinking water distribution systems. The controller leverages historical data to formulate and solve a constrained quadratic program (QP) without requiring an explicit system model.

2.1 Problem Setting and Notation

Let $u \in \mathbb{R}^m$ and $y \in \mathbb{R}^p$ denote the control input and sensor output signals. Where m, p are the dimensions of the actuators and sensors, respectively. A Hankel matrix of order L is defined by shifting the entries of a signal as shown in Eq. (1).

$$\mathcal{H}_L(u) = \begin{bmatrix} u_1 & \dots & u_{T-L+1} \\ \vdots & \ddots & \vdots \\ u_L & \dots & u_T \end{bmatrix} \tag{1}$$

The DeePC theory is based on a non-parametric representation of the system utilizing Hankel matrices constructed from measured input-output trajectories. The Hankel representation replaces the traditional parametric representation of an unknown dynamic system. Given a sufficiently rich dataset of input-output measurements, we stack them to build Hankel matrices for past and future sequences, see Eq. (2).

$$\begin{aligned} U_p \in \mathbb{R}^{mT_p \times N}, Y_p \in \mathbb{R}^{pT_p \times N} \\ U_f \in \mathbb{R}^{mT_f \times N}, Y_f \in \mathbb{R}^{pT_f \times N} \end{aligned} \tag{2}$$

Where T_p and T_f are parameters defined by the user to determine the duration of data sequences representing past and future horizons. $N = T - (T_p + T_f) + 1$ is the number of columns in each matrix. According to [Coulson *et al.*, 2019], T_p is the number of steps backward required for state estimation of the system, and T_f is the length of our predictive horizon. The reader is referred to [Coulson *et al.*, 2019] for more details about these parameters and the conditions for sufficiently rich data.

Relying on the behavioral system theory [Willems *et al.*, 2005], the DeePC theory offers a linear surrogate representation for the dynamic system, where a solution (u_{ini}, y_{ini}, u, y) is considered a feasible solution if there exists a vector $g\mathbb{R}^{mT_p \times N}$ that satisfies the constraints in Eq. (3)

$$\begin{aligned} \min_{g,\ u \in \mathcal{U},\ y \in \mathcal{Y}} \quad & \|y - y_{ref}\|_Q^2 + \|u\|_R^2 + \lambda_g \|g\|_1 + \lambda_y \|y\|_1 \\ \text{s.t.} \quad & \begin{bmatrix} U_P \\ Y_P \\ U_f \\ Y_f \end{bmatrix} g = \begin{bmatrix} u_{\text{ini}} \\ y_{\text{ini}} \\ u \\ y \end{bmatrix} + \begin{bmatrix} 0 \\ \sigma_y \\ 0 \\ 0 \end{bmatrix} \end{aligned} \tag{3}$$

Where u_{ini}, y_{ini} are the latest T_p measured values, and $\sigma_y, \lambda_g, \lambda_y$ are regularization terms that enable the method to overcome nonlinear dynamics and uncertain noises of the system.

Although proven in varied control applications [Perelman and Ostfeld, 2025], the above formulation might struggle with a high-dimensional input-output space dense sampling resolution, resulting in huge Hankel matrices. Moreover, the water quality behavior is non-linear and noisy, affected by disturbances in consumer demands and source quality.

To overcome these challenges, we adopted the Null-space parameterization suggested by [Zhou *et al.*, 2024], reducing the dimension of the decision variable in every control iteration. Another modification from the original DeePC was to optimize the relative change in every time step rather than the absolute dosage rates, as proposed by [de Jong and Lazar, 2024]. Optimizing the dose increment Δu explicitly decouples rate-limit constraints and keeps the quadratic term confined to a low-dimensional null-space basis, yielding a much sparser, faster-solvable optimization problem.

2.2 DeePC Formulation

The past data matrices are vertically stacked to build the complete past input-output sequences matrix

$$\mathcal{G}_p = \begin{bmatrix} U_p \\ Y_p \end{bmatrix} \in \mathbb{R}^{(m+p)T_p \times N} \tag{4}$$

where m is the number of chlorine injectors, p is the number of sensors, and N is the number of data sequences with length of T_p. Each column of $\mathcal{G}_p$ is therefore a complete, past trajectory observed during the offline experiment.

Let $g_0 \in \mathbb{R}^N$ denote the minimum-norm consistency vector. That is, a unique weight vector that exactly reconstructs the most recent T_p sample via $\mathcal{G}_p g_0 = [u_{ini}, y_{ini}]$, thereby providing the data-consistent baseline for our future-trajectory predictions. Next, we continue to build a null space of $\mathcal{G}_p$ by introducing $\mathcal{N} \in \mathbb{R}^{N \times d}$. The columns of $\mathcal{N}$ form an orthonormal basis of the null space of $\mathcal{G}_p$, such that $\mathcal{G}_p \mathcal{N} = 0$ and $\mathcal{N}\mathcal{N} = \mathcal{I}_d$. Where $d = dim[null(\mathcal{G}_p)]$, therefore d represents the number of independent "free directions" that leave the past unchanged.

Additionally, we introduce the vector $z \in \mathbb{R}^d$ as the null space coefficient vector. Each entry of z scales one of these free directions, so that $g = g_0 + \mathcal{N}z$ adjusts only the future part of the trajectory while satisfying the measured past exactly.

After constructing the minimum-norm vector g_0, we can use the future Hankel blocks U_f, Y_f to obtain the baseline predictions $(\bar{u}_f, \bar{y}_f)$. These baseline trajectories can be seen as the "nominal" trajectories in the sense that they reflect what would occur if the controller applied no new action, yet they are already guaranteed to honor the dynamics embedded in the training data and to match the freshly observed past exactly. Shaping the future behavior, we utilize the fact that any vector in the null space of $\mathcal{G}_p$ leaves the past untouched. Choosing a vector $z \in \mathbb{R}^d$ and adding $\mathcal{N}z$ to g_0 yields an augmented weight $g = g_0 + \mathcal{N}z$ with the same past but a modified future, Eq. (5).

$$U_f = \bar{u}_f + U_f \mathcal{N} z, \qquad Y_f = \bar{y}_f + Y_f \mathcal{N} z \tag{5}$$

Where the terms $U_f \mathcal{N} z$ and $Y_f \mathcal{N} z$ represent the change from the baseline values, allowing the controller with relative changes

With the above notation, we end up with the following optimization problem that is to be solved in every iteration to determine the chlorine injections for the next horizon.

$$\begin{aligned} \min_{z,\Delta u, s, s_u} \quad & \lambda_g \|z\|^2 + (\lambda_{u,\text{dev}} + \lambda_{u,\text{dose}}) \|\Delta u\|_1 \\ & + \lambda_y \|s\|_1 + \lambda_{u,\text{slack}} \|s_u\|_1 \\ \text{s.t.} \quad & \Delta u = U_f \mathcal{N} z \\ & 0 \leq \Delta u \leq u_{rate}^{max} \\ & u_{min} \leq \bar{u}_f + \Delta u + s_u \leq u^{max} \\ & y_{min} \leq \bar{y}_f + Y_f \mathcal{N} z - s \\ & \bar{y}_f + Y_f \mathcal{N} z + s \leq y^{max} \\ & s, s_u \geq 0 \end{aligned} \tag{6}$$

2.3 Hankel Matrix Generation (Offline Phase)

The first step to implement the above control framework is to construct proper Hankel matrices that capture the system dynamics. This stage is done offline by running simulations with various control trajectories. The chlorination trajectories for these simulations were generated randomly based on engineering judgment of what would be reasonable dosage rates. For example, the main booster at the DMA entrance will have the highest rates. The trajectories are split into the past, future blocks U_p, U_f, Y_p, Y_f to construct $\mathcal{G}_p$ and later compute its null space basis.

2.4 Execution Strategy

The real-time control is done within a predictive control framework, where in every w time steps an optimization problem is solved to determine the control policy for the next horizon. Since chlorine decay dynamics are characterized by time delays between injection to measured response, we wanted to not solve a new problem in every time step but give the system time to respond to a new policy and update only after changes were measured in the sensors. Furthermore, given that solving each optimization problem takes about a few dozen seconds, it will be impossible to solve a new problem with the 5 minutes steps simulations. By setting $w = 60$, a new policy is generated every 60 time steps, meaning every 5 hours, which is a reasonable delay time for chlorine in systems similar to the competition case study [Vrachimis *et al.*, 2024]. The strategy chosen the controller stores the optimized control plan u_f and sequentially applies its actions over a fixed time horizon. If the stored plan expires, a new QP is solved.

The DeePC policy is backed up by a low-level fallback controller that guarantees continued operation whenever the on-line QP is declared infeasible or exceeds its time budget. The fallback controller designed as a basic Proportional Integrated Derivative (PID) tuned to hold a 0.30 mg/L concentration at all sensors. The supervisory logic hands control back to DeePC as soon as a feasible QP solution is available, thus providing a provably safe transition between learning-based and classical control modes.

Results

The proposed method depends in many parameters, starting from how the train data (constant Hankel matrices) is generated, followed by the dimensions of T_p and T_f, the regularization terms, and the wait time between consecutive optimization solutions. Due to a lack of time to investigate different configurations, we used engineering judgment with some trial and error runs. Nevertheless, a disclaimer is made here that the algorithm may not be optimized to fulfill the competition objectives.

From exploitive analysis of the network we found that some nodes will always have chlorine residuals of 0, these are dead end branches with no consumption therefore no new water flowing to these nodes that remains with the initial quality value. Furthermore, the network topology is such that some nodes are kept with very low concentrations even when injecting large amounts of chlorine, which diminishes the effectiveness of the algorithms.

Figure 1 presents example of input-output trajectories of the proposed method for scenario 8 across 500 steps. Unfortunately the results does not look promising, it seems that the

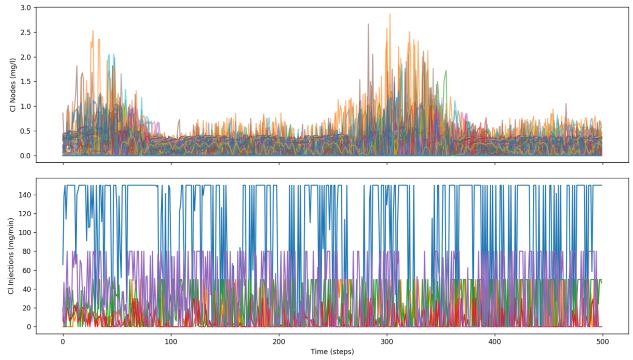

Figure 1: Example simulation results for scenario 8

proposed method could not learn the system dynamics and during most of the time, the chlorination policy is similar to what known as "Bang-Bang control".

The actuators increase until they hit their upper bound, then decreasing fast until hitting the lower bound and so forth. The impact of the consumption is very clear, where during off-peak consumption periods the chlorine residuals increasing dramatically above the desired upper bound of 0.4 mg/L. The proposed approach failed to prevent this behavior by minimizing the injections.

3 Summary

The paper proposes a data-enabled predictive control (DeePC) strategy for the IJCAI-2025 Drinking Water Chlorination Challenge, reconstructing network dynamics from past input-output data arranged in Hankel matrices and solving a null-space quadratic program to generate future chlorine injection profiles that minimize chemical use while meeting safety limits and infection-risk objectives. Key contributions include the DeePC-based optimizer, explicit actuator/sensor and slack constraints, and a hybrid architecture that hands control to a PID fallback whenever the on-line QP is infeasible or exceeds time limits. The optimization is resolved only every five hours to accommodate chlorine transport delays and to recycle previously computed trajectories, reducing runtime overhead. Preliminary simulations reveal that, under the scant configuration effort possible, the controller frequently lapses into bang-bang dosing and overshoots residual limits; the authors stress that these limitations stem from minimal tuning time and that the DeePC formulation itself may still need substantial refinement before it can meet the challenge objectives.

Ethical Statement

There are no ethical issues.

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