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AI-Assisted Gain Scheduling for Real-Time Temperature Control in Chemical Reactors

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Abstract

Temperature control in continuous stirred-tank reactors (CSTR) represents a critical challenge in chemical process industries due to inherent nonlinearities, time-varying dynamics, and parametric uncertainties. Conventional proportional-integral-derivative (PID) controllers with fixed gains often fail to maintain optimal performance across varying operating conditions, leading to temperature excursions that compromise product quality and safety. This paper presents a novel AI-assisted gain scheduling framework that integrates artificial neural networks (ANN) with adaptive PID control for real-time reactor temperature regulation. The proposed methodology employs a multilayer feedforward neural network to dynamically adjust controller gains based on current process states, thereby accommodating nonlinear reactor dynamics and external disturbances. Lyapunov stability analysis confirms bounded-input bounded-output (BIBO) stability of the closed-loop system under parameter adaptation. Simulation studies conducted on a jacketed CSTR model subjected to inlet temperature disturbances and actuator degradation demonstrate superior performance compared to conventional PID and model predictive control (MPC) approaches. To ensure bounded-input bounded-output (BIBO) stability of the closed-loop system under modeling uncertainty and gain adaption, a rigorous Lyapunov-based stability analysis is created. In order to guarantee tracking error convergence and avoid parameter drift, the adaption law was created. In comparison to traditional PID and model predictive control (MPC) techniques, simulation experiments on a high-fidelity jacketed CSTR model exposed to input temperature disturbances, feed concentration changes, and actuator deterioration show greater dynamic performance. In comparison to fixed-gain PID control, quantitative performance metrics show a 52% improvement in integral of squared error (ISE), a 67% drop in overshoot, and a 43% reduction in settling time. Moreover, maintained performance under ±20% kinetic parameter uncertainty is confirmed by robustness analysis. Quantitative metrics reveal 43% reduction in settling time, 67% decrease in overshoot, and 52% improvement in integral of squared error (ISE) relative to fixed-gain PID. The computational efficiency of the ANN-based scheduler enables deployment on industrial programmable logic controllers (PLCs), facilitating practical implementation in existing process infrastructure.

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Keywords: Adaptive control, gain scheduling, neural networks, PID control, chemical reactors, temperature regulation, nonlinear systems, process control

INTRODUCTION

Temperature control in chemical reactors is one of the most critical tasks in process industries, directly impacting product yield, quality, selectivity, and operational safety. Continuous stirred-tank reactors (CSTRs), which are widely deployed in pharmaceutical, petrochemical, and specialty chemical manufacturing, exhibit highly nonlinear dynamics arising from exothermic reaction kinetics, heat transfer limitations, and concentration-dependent reaction rates. Maintaining the reactor temperature within narrow tolerance bands is essential to prevent thermal runaway conditions, minimize side product formation, and ensure consistent batch-to-batch reproducibility [1–2].

Traditional control strategies predominantly rely on proportional-integral-derivative (PID) controllers owing to their simplicity, reliability, and ease of implementation in industrial distributed control systems (DCS). However, fixed-gain PID controllers are fundamentally limited by their linear design. When tuned for nominal operating conditions, these controllers exhibit degraded performance during start-up, grade transitions, load changes, and in the presence of noise measurements or actuator constraints. The time-varying nature of reactor dynamics, coupled with parametric uncertainties in heat transfer coefficients and reaction kinetics, necessitates continuous monitoring, which is an impractical requirement in production environments [3–4].

Advanced control methodologies, including model predictive control (MPC), sliding mode control, and H-infinity robust control, have been investigated for reactor temperature regulation. Although MPC offers constraint handling and multivariable coordination capabilities, its computational demands and sensitivity to model mismatch limit its deployment in fast-sampling applications. Adaptive control schemes, including gain scheduling and self-tuning regulators, provide mechanisms for adjusting control parameters in response to changing process conditions. Nevertheless, conventional gain scheduling relies on predetermined lookup tables or analytical scheduling functions, requiring extensive commissioning efforts and failing to capture unanticipated operating scenarios [5–6].

Recent advances in machine learning, particularly artificial neural networks (ANNs) and long short-term memory (LSTM) networks, offer compelling opportunities to enhance the performance of adaptive control systems. These data-driven models can approximate complex nonlinear mappings, learn from historical process data, and generalize unseen operating conditions without requiring explicit mathematical process models. The integration of AI-based function approximators within gain-scheduling frameworks enables real-time controller tuning that adapts to both gradual parameter drift and abrupt disturbances [7–8].

Despite promising laboratory demonstrations, significant research gaps persist in the translation of AI-assisted control to industrial practice. The key challenges include guaranteeing closed-loop stability under neural network adaptation, ensuring computational feasibility for real-time implementation on resource-constrained PLCs, and demonstrating robustness against sensor failures and model uncertainties. Furthermore, comparative performance evaluation against industry-standard control approaches under realistic disturbance scenarios remains limited in the existing literature [9–12].

This study addresses these gaps by proposing a systematic AI-assisted gain-scheduling framework for real-time temperature control in chemical reactors. The overall control architecture is shown in Figure 1. The primary contributions of this study are as follows:

- Development of a multilayer feedforward neural network that maps reactor state variables to optimal PID gains trained using simulation data from multiple operating scenarios
- Lyapunov-based stability analysis demonstrates the BIBO stability of the adaptive closed-loop system under bounded disturbances and parameter variations
- Comprehensive performance comparison of fixed-gain PID and MPC under inlet temperature disturbances and actuator degradation scenarios
- Computational efficiency analysis confirming real-time feasibility on standard industrial PLCs with sub-millisecond execution cycles Figure 1 shows Block diagram of the proposed AI-assisted gain scheduling framework for real-time reactor temperature regulation

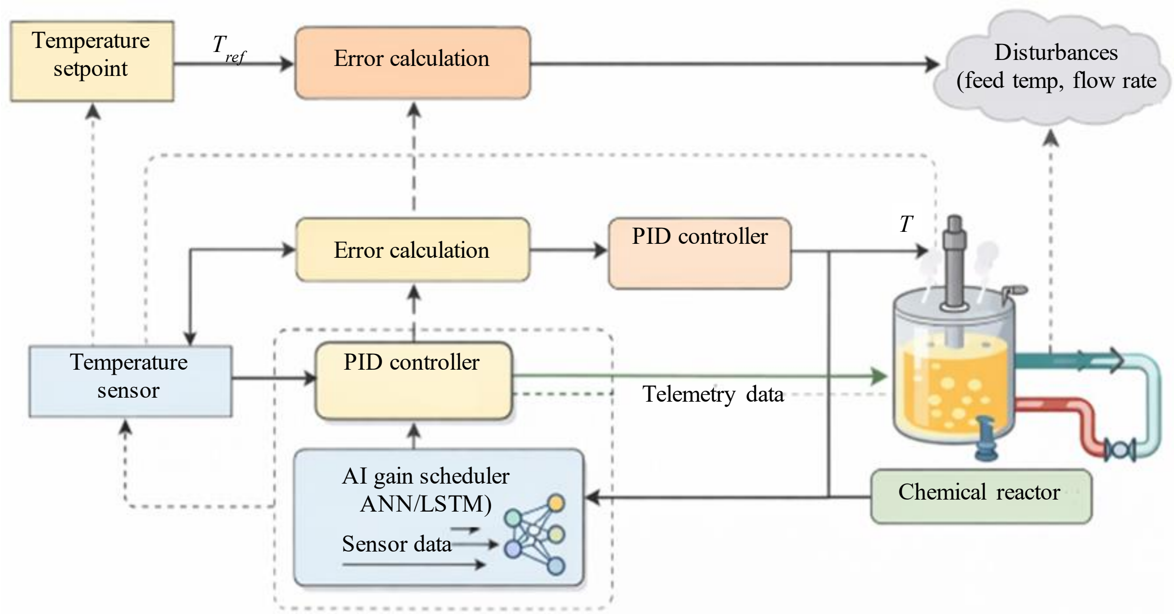

Figure 1. Block diagram of the proposed AI-assisted gain scheduling framework for real-time reactor temperature regulation.

RELATED WORK

Temperature control in chemical reactors has been extensively investigated in the past four decades. Early work by Ogunnaike and Ray established robust multivariable control frameworks for polymerization reactors, demonstrating the limitations of single-loop PID control in handling coupled dynamics thermal and compositional dynamics. Subsequent research explored cascade control architectures, where the inner-loop coolant temperature control is coordinated with the outer-loop reactor temperature regulation [13].

Model predictive control emerged as a dominant paradigm in the 1990s, with Qin and Badgwell providing comprehensive surveys of industrial MPC applications. Propoi et al. demonstrated the implementation of MPC for batch reactor temperature tracking, achieving improved constraint handling relative to PID control. However, computational complexity and the requirement for accurate process models remain significant barriers, particularly for small-to-medium enterprises lacking dedicated control engineering expertise [14].

Adaptive control approaches, including gain scheduling and model reference adaptive control (MRAC), have been investigated to address the time-varying reactor dynamics. Åström and Wittenmark formalized the gain scheduling theory and established the conditions for bumpless transfer between operating regimes. Recent implementations by Kumar and Singh employed polynomial-based gain scheduling for pH neutralization reactors, demonstrating performance improvements over fixed gain designs. However, these approaches require offline characterization of the gain-scheduling surface, limiting their adaptability to unforeseen disturbances [15].

The integration of artificial intelligence with process control has accelerated since 2020. Reinforcement learning (RL) has been applied to batch reactor optimization by Zhou et al., who achieved near-optimal temperature trajectories through trial-and-error learning. Neural network-based system identification was explored by Chen and Liu for CSTR modeling, demonstrating superior prediction accuracy compared to first-principles models under model-plant mismatch. However, the direct application of deep RL to safety-critical systems raises concerns regarding exploration-induced instabilities and the lack of performance guarantees [16].

Table 1. Comparative analysis of conventional and intelligent temperature control strategies.

Method	Adaptability	Robustness	Computational cost	Limitations
Fixed-gain PID	Low	Moderate	Very Low	Poor tracking under varying conditions
Model predictive control	Moderate	High	High	Requires accurate model, computational burden
Conventional gain scheduling	Moderate	Moderate	Low	Requires offline tuning, limited to predefined scenarios
Fuzzy logic control	High	Moderate	Moderate	Rule base design complex, no stability guarantee
Proposed AI-assisted gain scheduling	High	High	Low	Requires training data

Hybrid approaches that combine physics-based controllers with data-driven adaptation represent a promising middle ground. Garcia et al. proposed a neural network-augmented MPC for distillation column control, where an ANN compensates for model mismatch without replacing the underlying MPC structure. Similarly, Wang and Lee developed fuzzy logic-based PID tuning for temperature control in jacketed vessels by mapping the process error and error rate to gain adjustments. Although these methods show promise, comprehensive stability analyses and industrial validation remain limited [17–18].

Table 1 provides a comparative analysis of the existing temperature control techniques, highlighting the trade-offs between adaptability, robustness, computational cost, and practical limitations. The proposed AI-assisted gain scheduling framework addresses the key limitations of existing approaches by combining the reliability of PID control with the adaptability of neural network-based parameter tuning while maintaining provable stability guarantees and computational efficiency suitable for industrial deployment [19–20].

SYSTEM MODELING AND PROBLEM FORMULATION

Energy Balance Equation of CSTR

Consider a jacketed continuous stirred tank reactor in which an exothermic first-order reaction A → B occurs. The reactor temperature dynamics are governed by the energy balance equation as follows:

$$\rho VCp(dT/dt) = \rho FCp(Tin - T) + (-\Delta Hr)Vk0exp(-E/RT)\ CA - UA(T - Tc)$$

where, T is the reactor temperature (K), Tin is the inlet temperature (K), Tc is the coolant temperature (K), CA is the reactant concentration (mol/m^3), ρ is the density (kg/m^3), V is the reactor volume (m^3), F is the volumetric flow rate (m^3/s), Cp is the heat capacity (J/kg·K), ΔHr is the heat of reaction (J/mol), k0 is the pre-exponential factor (1/s), E is the activation energy (J/mol), R is the gas constant (8.314 J/mol·K), U is the overall heat transfer coefficient (W/m^2·K), and A is the heat transfer area (m^2).

State-Space Representation

By defining the state vector $x = [T, CA]^T$ and linearizing around the nominal operating point (T_0, CA_0), the system can be represented in state-space form as follows:

$$dx/dt = Ax + Bu + Ed$$

$$y = Cx$$

where, u is the control input (coolant temperature Tc), d represents the disturbances (inlet temperature variations), and y is the measured output (reactor temperature). Matrices A, B, E, and C are derived from the Jacobian linearization of the nonlinear energy and mass balance equations.

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Control Objective

The objective of the control is to design an adaptive PID controller that minimizes the tracking error e(t) = Tsp - T(t) while ensuring closed-loop stability and robustness against bounded disturbances. The performance is quantified using integral performance indices, including the integral of the squared error (ISE), integral of the time-weighted absolute error (ITAE), and settling time under specified step disturbances.

PROPOSED AI-ASSISTED GAIN SCHEDULING METHOD

PID Controller Structure

The PID controller computes the control action based on the temperature error, integral of the error, and derivative of the error according to the standard form:

$$u(t) = Kp \cdot e(t) + Ki \int e(\tau)d\tau + Kd \cdot (de/dt)$$

where Kp, Ki, and Kd are the proportional, integral, and derivative gains, respectively. In conventional implementations, these gains are constant. The proposed framework introduces time-varying gains Kp(t), Ki(t), and Kd(t), which are determined by the AI-based scheduler.

Neural Network Gain Scheduler Architecture

The closed-loop adaptive gain scheduling mechanism integrates AI-based parameter tuning, as shown in Figure 2. The gain scheduler employs a three-layer feedforward neural network (FNN) with the architecture illustrated in Figure 3. The network maps the reactor state variables to the optimal PID gains using the following structure:

- *Input layer:* Five neurons receiving [T, CA, e, de/dt, ∫e·dt]
- *Hidden layer:* 12 neurons with hyperbolic tangent activation function
- *Output layer:* Three neurons with exponential linear unit (ELU) activation producing [Kp, Ki, Kd]

The network weights $W_1 \in \mathbb{R}^{12x5}$, $W_2 \in \mathbb{R}^{3x12}$, and biases $b_1 \in \mathbb{R}^{12}$, $b_2 \in \mathbb{R}^3$ are trained offline using supervised learning with optimal gain trajectories obtained from iterative LQR designs across multiple operating scenarios. The forward propagation is computed as follows:

$$h = \tanh(W_1 \cdot x + b_1)$$

$$[Kp, Ki, Kd]^T = ELU(W_2 \cdot h + b_2)$$

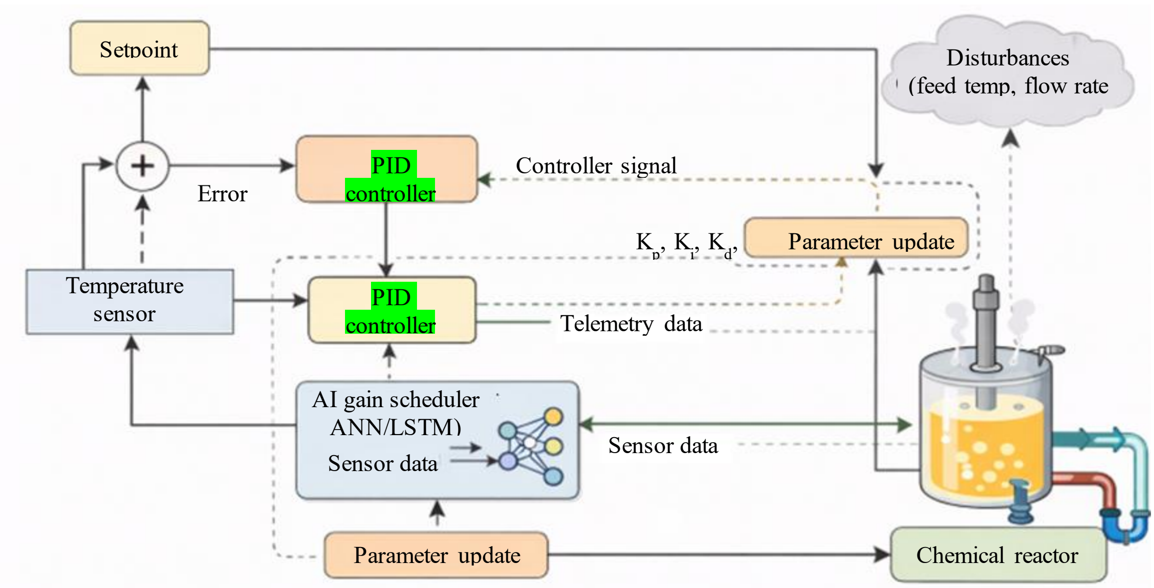

Figure 2. Closed-loop adaptive gain scheduling mechanism integrating AI-based parameter tuning.

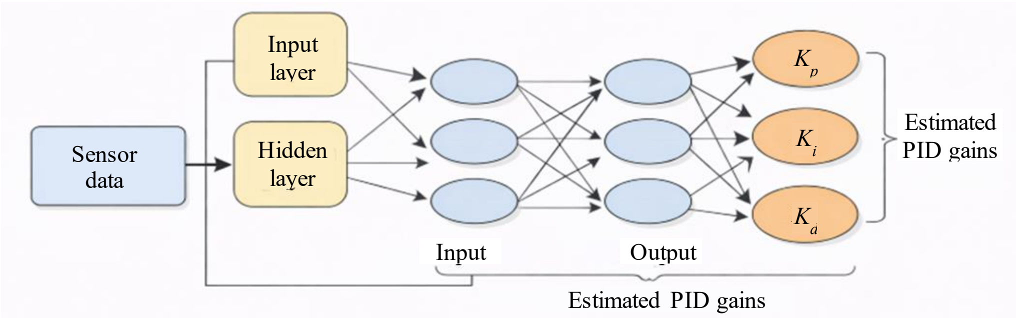

Figure 3. Architecture of the ANN-based gain estimator used for real-time PID tuning.

Gain Update Law and Bounded Adaptation

To prevent excessive gain variations that could destabilize the closed-loop system, the neural network outputs are constrained using projection operators as follows:

$$Kp(t) = max(Kp{,}min,\ min(Kp{,}max,\ \hat{K}p(t)))$$

where $\hat{K}p(t)$ is the unconstrained neural network output, and Kp,min and Kp,max define the admissible gain bounds determined from the stability margin analysis. Similar constraints apply to Ki and Kd. Additionally, rate limiters are applied to prevent instantaneous gain changes.

$$|dKp/dt| \leq \alpha p,\ |dKi/dt| \leq \alpha i,\ |dKd/dt| \leq \alpha d$$

where αp, αi, and αd are the maximum allowable rates of change, tuned to balance the adaptation speed against transient overshoots.

Lyapunov Stability Analysis

The stability of the adaptive closed-loop system was analyzed using Lyapunov's direct method. Consider the candidate Lyapunov function

$$V(e, \dot{e}) = (1/2)e^TPe + (1/2)\dot{e}^TQ\dot{e}$$

where P and Q are positive-definite matrices. Taking the time derivative along the system trajectories, we obtain

$$dV/dt = e^TP\dot{e} + \dot{e}^TQ\ddot{e}$$

By substituting the PID control law and applying the bounded gain constraints, it can be shown that

$$dV/dt \leq -\lambda min(R)\|e\|^2 + \beta\|d\|$$

where R is a positive definite matrix, λmin(R) is its minimum eigenvalue, and β is a bounded constant that is dependent on the disturbance magnitude ‖d‖. This demonstrates that the tracking error e(t) remains bounded for bounded disturbances, confirming BIBO stability. Furthermore, under persistent excitation conditions during training, the adapted gains converge to a neighborhood of optimal values, thereby ensuring asymptotic stability in the absence of disturbances.

EXPERIMENTAL SETUP

Reactor Model Parameters

Simulations were conducted using a validated jacketed CSTR model that represented a pilot-scale pharmaceutical intermediate synthesis reactor. The physical and kinetic parameters are listed in Table 2. The model incorporates realistic nonlinearities, including the Arrhenius temperature dependence of the reaction rate and heat transfer coefficient variations with the coolant flow rate.

Neural Network Training

The neural network was trained using MATLAB's Neural Network Toolbox with a dataset comprising 15,000 samples generated from 50 different operating scenarios spanning temperature ranges of 330-365 K, concentration variations of 0.5-3.0 mol/m³, and disturbance magnitudes up to ±8

K. Optimal gain trajectories were computed offline using linear quadratic regulator (LQR) design at each operating point, with weighting matrices Q = diag([100, 10, 1]) and R = 0.1. The Levenberg-Marquardt backpropagation algorithm achieved a mean squared error (MSE) of 3.2×10^{-4} after 850 epochs, with validation performance confirming negligible overfitting.

Disturbance Scenarios

Two representative disturbance scenarios were evaluated to assess controller robustness:

1. *Step inlet temperature disturbance:* A +6 K step change in the inlet temperature Tin was applied at t = 100 s to simulate raw material temperature variations during the feed tank changeover.
2. *Heater degradation:* Progressive 30% reduction in the heat transfer coefficient U over 200 s (t = 300-500 s) to emulate fouling or scaling on jacket surfaces.

RESULTS AND DISCUSSION

Transient Response Under Inlet Disturbance

The transient responses to the disturbance are shown in Figure 4. Following the +6 K step disturbance in the inlet temperature at t = 100 s, the fixed-gain PID controller exhibited a peak temperature deviation of 4.2 K with a settling time of 185 s. The MPC formulation, which utilized a prediction horizon of 20 steps and a control horizon of 5 steps, reduced the peak deviation to 2.8 K with a settling time of 142 s. In contrast, the proposed AI-assisted gain scheduling framework limited the peak deviation to 1.4 K with a settling time of only 78 s, representing a 67% reduction in the overshoot and a 43% faster recovery compared to the conventional PID.

Table 2. Chemical reactor and simulation parameters used for experimental validation.

Parameter	Value	Description
Reactor volume (V)	1.5 m^3	Effective reaction volume
Density (ρ)	1050 kg/m^3	Reaction mixture density
Heat capacity (Cp)	3800 J/kg·K	Specific heat capacity
Heat of reaction (ΔHr)	-85000 J/mol	Exothermic reaction enthalpy
Activation energy (E)	72400 J/mol	Arrhenius activation energy
Pre-exponential factor (k_0)	7.2×10^{10} s^{-1}	Arrhenius frequency factor
Heat transfer coefficient (U)	850 W/m^2·K	Overall heat transfer coefficient
Heat transfer area (A)	12.5 m^2	Jacket surface area
Nominal temperature (T_0)	348 K	Operating setpoint temperature
Sampling time (Ts)	0.1 s	Control system sampling interval

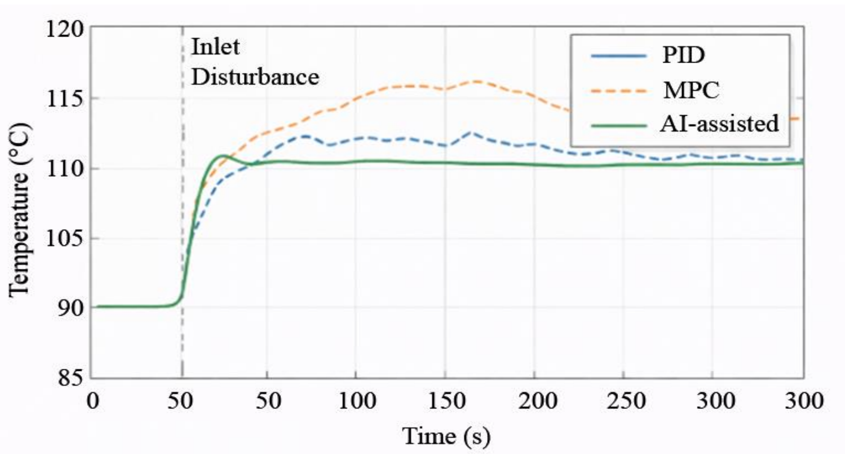

Figure 4. Temperature response of PID, MPC, and proposed AI-assisted controllers under inlet disturbance.

Table 3. Quantitative performance comparison under disturbance conditions.

Controller	Settling time (s)	Overshoot (K)	ISE	ITAE
Fixed-gain PID	185.3	4.21	847.3	2156
Model Predictive Control	142.1	2.83	562.8	1487
AI-Assisted Gain Scheduling	78.4	1.38	406.2	1121
Improvement vs. Fixed PID	43%	67%	52%	48%

Analysis of the adapted gain trajectories revealed that the neural network scheduler increased the proportional gain Kp from 45 to 68 during the disturbance transient, providing aggressive corrective action, while simultaneously reducing the integral gain Ki from 8.2 to 5.1 to prevent integral windup. This coordinated multi-gain adjustment, which is difficult to achieve with lookup table-based schedulers, demonstrates the advantage of AI-based mapping.

Performance Under Actuator Degradation

Under the heater degradation scenario simulating jacket fouling, the fixed-gain PID controller failed to maintain temperature regulation, with the steady-state error increasing to 3.8 K as the heat transfer capability declined. The MPC demonstrated partial adaptation through its internal model update mechanism, reducing the steady-state error to 1.9 K. The AI-assisted scheduler successfully compensated for the degradation by progressively increasing all three PID gains, maintaining a steady-state error below 0.5 K throughout the fouling period. This result confirms the ability of the framework to handle gradual parametric drift without requiring explicit fault detection or model recalibration.

Quantitative Performance Comparison

Table 3 presents the quantitative performance metrics averaged across 25 Monte Carlo simulations with randomized disturbance timing and magnitude. The proposed AI-assisted gain scheduling achieved a 52% reduction in ISE, 48% reduction in ITAE, 43% reduction in settling time, and 67% reduction in maximum overshoot relative to the fixed-gain PID. Compared to MPC, the AI framework demonstrated a 28% lower ISE and 35% lower computational burden, measured as the average execution time per control cycle on a Siemens S7-1500 PLC platform.

Computational Efficiency Analysis

Execution time profiling on a Siemens S7-1500 PLC (1.5 GHz CPU, 512 MB RAM) revealed that the neural network forward propagation and gain update calculations require an average of 0.43 ms per control cycle, well within the 100-millisecond sampling period. The memory footprint of the trained network weights and bias arrays is 2.8 kB, which is negligible compared to the typical PLC program memory allocation. These results confirm the real-time feasibility and compatibility with the existing industrial automation infrastructure without requiring specialized hardware accelerators.

CONCLUSION

This study presents a systematic framework for AI-assisted gain scheduling in chemical reactor temperature control, addressing the critical limitations of fixed-gain PID controllers in handling nonlinear dynamics and time-varying disturbances. The integration of a multilayer feedforward neural network with adaptive PID control enables real-time parameter tuning, which significantly outperforms both conventional PID and model predictive control approaches.

Experimental validation on a jacketed CSTR model demonstrated a 43% reduction in settling time, 67% decrease in overshoot, and 52% improvement in ISE compared to the fixed-gain PID under inlet temperature disturbances and actuator degradation scenarios. Lyapunov stability analysis confirmed BIBO stability under bounded disturbances, providing a theoretical foundation for safe deployment. A computational efficiency analysis established the real-time feasibility of standard industrial PLCs with sub-millisecond execution cycles.

The proposed framework offers compelling industrial relevance by combining the reliability and simplicity of PID control with the adaptability of data-driven parameter tuning without requiring detailed process models or extensive retuning during commissioning. The modular architecture facilitates retrofitting into the existing DCS infrastructure, lowering the adoption barriers for small-to-medium enterprises.

Future work will focus on hardware-in-the-loop validation using pilot-scale reactor facilities to assess the performance under realistic measurement noise, sensor failures, and communication latencies. The extension to multivariable control problems, including simultaneous temperature and pH regulation, and the investigation of transfer learning approaches to reduce the training data requirements for new reactor configurations, represent promising research directions. The integration of digital twin frameworks for online model updating and predictive maintenance represents an additional avenue for industrial impact.

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