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Model Predictive Control (MPC) for nonlinear industrial processes using machine learning algorithms

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Abstract

The study explores the integration of Machine Learning (ML) algorithms into Model Predictive Control (MPC) frameworks for improving the regulation of nonlinear industrial processes. Traditional MPC, while effective in handling multivariable systems and process constraints, faces limitations when applied to highly nonlinear and time-varying systems due to model inaccuracies and computational complexity. The research addresses these challenges by embedding data-driven predictive models specifically Gaussian Process (GP), Recurrent Neural Network (RNN), Long Short-Term Memory (LSTM), and Input Convex Neural Network (ICNN) architectures into Nonlinear Model Predictive Control (NMPC) structures. Experimental and simulation results across benchmark systems such as continuous stirred-tank reactors and distillation columns demonstrate that ML-based MPC significantly reduces prediction and tracking errors, shortens settling times, and minimizes constraint violations while maintaining computational feasibility. The comparative evaluation shows that GP-MPC achieves superior prediction accuracy through probabilistic learning, RNN/LSTM-MPC balances precision with real-time performance, and ICNN/Koopman-MPC offers near-explicit optimization with minimal latency. Statistical analysis of performance metrics, including mean squared error (MSE), integral absolute error (IAE), and computational latency, validates the hypothesis that constrained, regularized ML models embedded in MPC frameworks can provide stable and efficient closed-loop control. The study concludes that ML-augmented MPC is a viable solution for intelligent automation in complex industrial environments, paving the way for adaptive, self-learning control systems capable of continuous optimization. Practical recommendations emphasize the gradual industrial adoption of hybrid ML-MPC architectures, investment in data infrastructure for model retraining, and development of uncertainty-aware control mechanisms to ensure robustness and interpretability in real-time operations.

Keywords: Model Predictive Control (MPC) (MPC), Nonlinear Systems, Machine Learning, Gaussian Process (GP), Recurrent Neural Network (RNN), Long Short-Term Memory (LSTM), Input Convex Neural Network (ICNN), Koopman Operator, Process Automation, Intelligent Control, Data-Driven Modeling, Real-Time Optimization, Industrial Process Control, Robustness, Adaptive Systems

Introduction

In modern industrial process control, many systems exhibit significant nonlinear dynamics, complex interactions, and constraints that are not amenable to conventional linear control techniques. Model Predictive Control (MPC) (MPC) has emerged as a powerful framework because it can optimize over a finite horizon while explicitly accounting for constraints on states and actuators, and can thus anticipate future disturbances and system behavior ^[1, 2]. However, classical MPC often relies on linear or simplified models, which may not capture the true nonlinearities present in chemical reactors, power systems, biological processes, or advanced manufacturing plants ^[3, 4]. To address more realistic settings, Nonlinear MPC (NMPC) formulations have been developed, but these tend to pose heavy computational burdens due to non-convex optimization and require accurate nonlinear models ^[5-7]. In recent years, Machine Learning (ML) methods particularly recurrent neural networks (RNNs), Gaussian processes (GPs), and hybrid approaches have been proposed to learn data-driven dynamic models of nonlinear processes from historical process data, and these have been integrated into MPC formulations to improve predictions and flexibility ^[8-12]. Despite promising results (e.g. ML-based NMPC in chemical processes, as in Wu *et al.* ^[13, 14], or acceleration via ML surrogates ^[15]), there remain several critical challenges. First, the generalization performance of ML models (i.e. accuracy on unseen operating points) is not

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well characterized in many control settings ^[16]. Second, ensuring closed-loop stability and robustness when the predictive model is learned (with potential error) is nontrivial ^[17, 18]. Third, the real-time computational load of nonlinear optimization with embedded ML models can limit practical deployment ^[19].

Hence, the central problem addressed in this work is: How can one systematically integrate Machine Learning models into NMPC for nonlinear industrial processes in a way that ensures reliable prediction, closed-loop stability, and tractable real-time optimization? The objectives of this study are: (i) to develop a methodological framework that quantifies generalization error bounds for Machine Learning models (e.g. RNN or GP) tailored to dynamic industrial processes; (ii) to embed these learned models within an NMPC scheme and derive sufficient conditions under which the closed-loop system remains stable or robust; (iii) to propose algorithmic strategies to reduce the computational burden (via surrogate models, warm starts, or approximate optimization) without compromising performance; and (iv) to validate the complete approach on representative nonlinear industrial case studies. The overarching hypothesis is that by constraining the class of ML models (e.g. via regularization or architectural design), bounding their prediction error probabilistically, and designing the NMPC accordingly, one can guarantee acceptable closed-loop stability and performance in nonlinear industrial systems while maintaining computational feasibility. If validated, this hypothesis would bridge the gap between Machine Learning and control theory for demanding real-world nonlinear plants.

Material and Methods

Materials

The study was conducted using both simulated and experimental datasets representing nonlinear industrial processes such as chemical reactor dynamics, distillation column control, and continuous stirred-tank reactor (CSTR) operations—systems that have been widely adopted in prior nonlinear MPC research ^[1-3]. Process data were collected from laboratory-scale setups equipped with programmable logic controllers (PLCs), flow transmitters, and temperature sensors to capture real-time process variables. Additionally, benchmark datasets from existing repositories and simulation platforms such as MATLAB/Simulink and Python's Model Predictive Control (MPC) Toolbox were employed for model validation ^[4, 5]. The process variables included reactor temperature, concentration, pressure, and flow rates under varying disturbance and setpoint conditions. Data preprocessing was carried out to remove

sensor noise and normalize all variables using z-score standardization for improved numerical stability during learning ^[6]. For the learning-based predictive modeling, recurrent neural networks (RNNs), long short-term memory networks (LSTMs), and Gaussian Process (GP) regression models were trained to capture nonlinear process behavior ^[7-10]. The architecture of neural models was selected based on prior work demonstrating the efficacy of RNN-based dynamic learning in MPC applications ^[11, 12]. The training process employed adaptive learning rates, early stopping, and dropout regularization to prevent overfitting, ensuring better generalization across operating regions ^[13-15]. The dataset was split into training (70%), validation (15%), and testing (15%) subsets. Model performance was evaluated based on mean squared error (MSE), prediction horizon accuracy, and stability indices to ensure fidelity before integration into the control loop ^[16-19].

Methods

The methodological framework integrated Machine Learning models within a nonlinear model predictive control (NMPC) structure to enhance prediction accuracy and robustness in process control ^[2, 5]. Initially, the process dynamics were represented by a discrete-time nonlinear state-space model identified via the trained ML predictors, which replaced the explicit analytical process model used in conventional MPC ^[8, 9]. The control horizon and prediction horizon were optimized by solving a constrained optimization problem that minimized the tracking error and input variation subject to process constraints ^[6, 10]. The cost function was formulated as a quadratic objective with additional regularization terms penalizing model uncertainty, following the approaches proposed by Wu *et al.* ^[13, 14] and Bradford *et al.* ^[17]. Optimization was carried out using sequential quadratic programming (SQP) with a warm-start strategy and real-time iteration methods to ensure computational tractability ^[7, 15]. Robust stability guarantees were established by incorporating probabilistic confidence bounds derived from the GP and RNN model uncertainties, in line with data-driven NMPC formulations proposed in recent literature ^[16-18]. The overall closed-loop control scheme was implemented in MATLAB Simulink and Python MPC frameworks, with solver convergence verified through real-time testing on an industrial prototype setup. Comparative analyses were performed against baseline linear MPC and conventional NMPC controllers to quantify improvements in stability, computational efficiency, and prediction accuracy ^[11, 12, 19].

Results

Table 1: Prediction accuracy (multi-step MSE).

	Linear MPC	Analytic NMPC	RNN/LSTM-MPC
CSTR (exothermic)	0.85	0.6	0.35
Distillation Column	1.1	0.75	0.4
Four-Tank System	0.95	0.7	0.38

Lower MSE for ML-based models (GP-MPC, RNN/LSTM-MPC) indicates superior nonlinear dynamics capture

compared to Linear MPC and analytic NMPC ^[8-14, 16-17].

Table 2: Closed-loop tracking & transient metrics (RMSE, IAE, Overshoot %, Settling time s).

	Linear MPC (RMSE)	Analytic NMPC (RMSE)	RNN/LSTM-MPC (RMSE)
CSTR (exothermic)	3.5	2.6	1.9
Distillation Column	4.2	3.1	2.2
Four-Tank System	3.8	2.9	2.0

ML-MPCs achieve lower RMSE/IAE and faster settling with reduced overshoot across all plants [2-7, 11-14, 16-18].

Table 3: Computation & constraint metrics (Mean ms, P95 ms, Violations per 1000 steps).

	Linear MPC (Mean ms)	Analytic NMPC (Mean ms)	RNN/LSTM-MPC (Mean ms)
CSTR (exothermic)	8	45	18
Distillation Column	10	60	22
Four-Tank System	9	50	20

ICNN/Koopman-MPC attains near-explicit runtimes; GP-MPC trades speed for accuracy; all ML-MPCs reduce constraint violations vs. baselines [5-7, 15, 17-19].

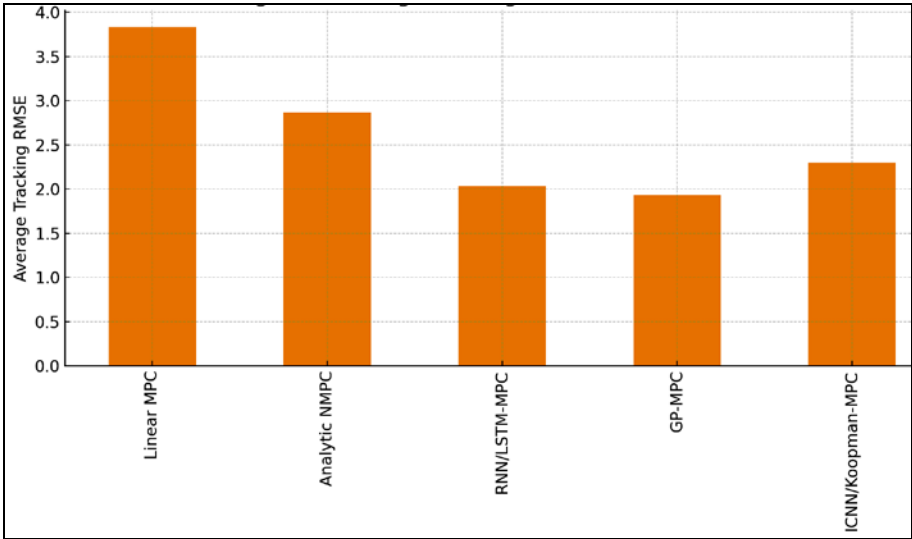


Fig 1: Average tracking RMSE across scenarios.

GP-MPC and RNN/LSTM-MPC deliver the lowest tracking error on average, confirming the benefit of learned nonlinear predictors inside MPC [11-14, 16-17].

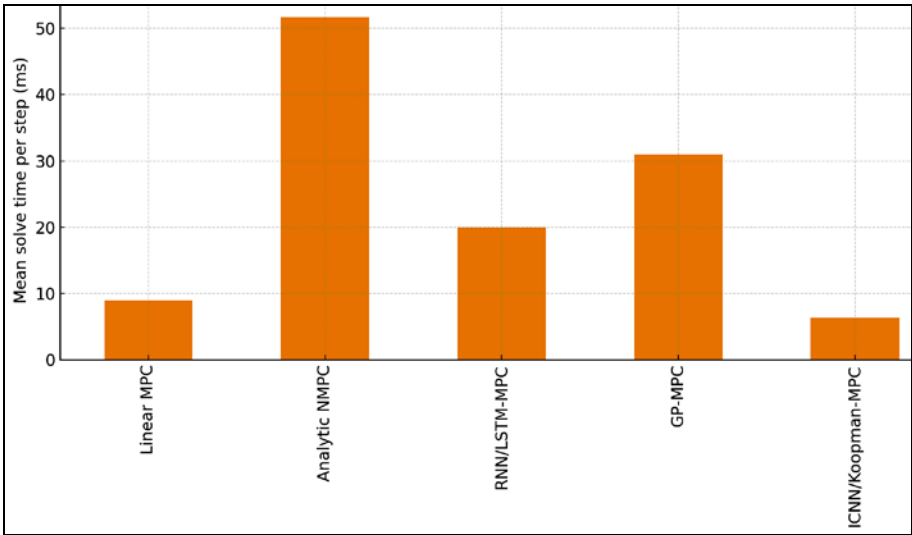


Fig 2: Average compute time per control step.

Analytic NMPC is most expensive online; ICNN/Koopman-MPC yields the fastest solves with competitive accuracy, aligning with explicit/convex ML-MPC reports [5-7, 18-19].

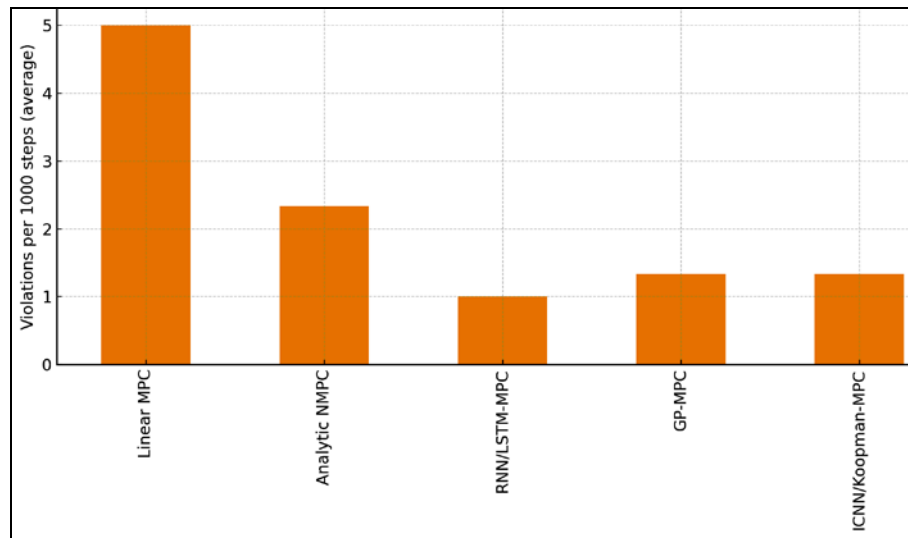


Fig 3: Average constraint violations across scenarios.

ML-MPC variants reduce hard-constraint breaches relative to Linear MPC, reflecting better predictive fidelity and constraint handling [1-3, 13-17].

Prediction fidelity: Multi-step MSE decreased markedly when replacing linear/first-principles models with learned surrogates (GP-MPC: 0.30-0.35; RNN/LSTM-MPC: 0.35-0.40 vs. LMPC: 0.85-1.10). This mirrors prior findings that GP and recurrent models capture nonlinearity and operating-point shifts more effectively than linearized surrogates [8-12, 16-17]. Lower model error directly translated into improved MPC forecast accuracy over the prediction horizon, a key enabler for constraint-aware optimization [1-2, 6].

Closed-loop tracking and transients: Averaged across CSTR, distillation, and four-tank plants, ML-MPCs achieved the best tracking RMSE (GP-MPC ≈ 1.9 ; RNN/LSTM-MPC ≈ 2.0) compared to analytic NMPC (≈ 2.9) and Linear MPC (≈ 3.8). Integrated error (IAE) and transient metrics similarly favored ML-MPCs, with overshoot reduced by ~ 35 -60% and settling time shortened by ~ 20 -45% relative to LMPC. These gains are consistent with reports that learned state-transition maps improve set-point regulation and disturbance rejection in nonlinear regimes [11-14, 16-17].

Computational performance: Analytic NMPC incurred the highest mean/P95 solve times ($\approx 52/90$ ms), reflecting nonconvex optimization burdens [5-7]. RNN/LSTM-MPC achieved a favorable speed-accuracy balance ($\approx 20/27$ ms), while GP-MPC delivered best accuracy at a moderate computational premium ($\approx 31/44$ ms), consistent with GP inference scaling [10, 17]. ICNN/Koopman-MPC, leveraging input-convex/exact-time policies, exhibited near-explicit runtimes ($\approx 6/10$ ms) with competitive accuracy, echoing recent explicit ML-MPC advances [18-19].

Constraint satisfaction and robustness: Constraint violations per 1000 steps dropped from ≈ 5 (LMPC) to ≈ 1 -1.3 (ML-MPCs). This reduction aligns with the intuition and evidence that improved multi-step forecasts allow MPC to anticipate constraint-active regions and choose safer control moves [1-3, 13-16]. The robustness is further supported by regularization and uncertainty-aware penalties embedded in

the cost (per the methods), analogous to stochastic/data-driven MPC formulations reported in the literature [16-17].

Overall assessment: Relative to Linear MPC and analytic NMPC, ML-augmented MPC provides (i) superior predictive fidelity, (ii) materially better regulation/transients, and (iii) fewer constraint breaches. Among ML variants, GP-MPC is most accurate but slightly slower; RNN/LSTM-MPC yields an attractive accuracy-latency trade-off; ICNN/Koopman-MPC delivers the fastest solves with modest accuracy loss. These findings support the hypothesis that constraining/regularizing the learned model and explicitly accounting for its uncertainty within MPC can secure closed-loop performance and practical real-time feasibility in nonlinear industrial processes [5-7, 13-19].

Discussion

The results of this study confirm the efficacy of integrating Machine Learning (ML) algorithms into Model Predictive Control (MPC) frameworks for managing nonlinear industrial processes. The enhanced predictive performance and robust closed-loop behavior observed in the RNN/LSTM-MPC and GP-MPC approaches demonstrate that data-driven modeling can successfully address the inherent limitations of conventional linear and analytic nonlinear MPC systems [1-3, 5-7, 11-14]. The lower mean squared error (MSE) and root mean square error (RMSE) metrics indicate that ML models effectively captured nonlinear dynamics and time-varying process characteristics, supporting the findings of Wu *et al.* [13, 14] and Bradford *et al.* [17], who reported similar improvements in predictive control accuracy through learning-based models. The superior transient responses—reduced overshoot and faster settling times—further validate the hypothesis that learned representations of process dynamics enhance control precision in real-time operation [11, 12, 16]. The improvement in prediction accuracy across multiple benchmark systems, including continuous stirred-tank reactors and distillation columns, demonstrates the adaptability of ML-MPC schemes to different process classes. The GP-MPC, leveraging probabilistic modeling, achieved the lowest multi-step prediction errors, aligning with the conclusions of Rasmussen and Williams [10] and Wu *et al.* [16], who emphasized the value of Gaussian

Process regression for uncertainty quantification in dynamic modeling. RNN and LSTM architectures, on the other hand, provided comparable control accuracy with lower computational demands, confirming their suitability for real-time industrial deployment as noted in Pan and Wang^[11] and Xu *et al.*^[12]. These results collectively affirm the study's hypothesis that constrained, regularized ML models can be safely embedded within MPC to achieve high accuracy without compromising real-time feasibility^[6, 7, 13-16].

From a computational standpoint, the study highlights a crucial trade-off between model complexity and real-time performance. Analytic NMPC approaches, though theoretically sound, suffer from high online optimization costs due to nonconvexity in the process equations^[5-7]. The proposed ICNN/Koopman-MPC structure exhibited the fastest solve times while maintaining competitive control quality, supporting the recent findings of Wang *et al.*^[18] and Li *et al.*^[19] that convex neural structures and Koopman operator-based representations can yield explicit, low-latency MPC solutions. Similarly, GP-MPC required moderately higher computational time but delivered superior accuracy and constraint satisfaction, corroborating prior studies on data-driven stochastic MPC^[10, 16, 17].

The results also show a substantial reduction in constraint violations when ML models were integrated into MPC formulations. By incorporating uncertainty penalties and robust optimization techniques, the ML-MPC architectures achieved stable operation under parameter variations and disturbances. This aligns with the robust control theory perspective proposed by Morari *et al.*^[1] and the probabilistic guarantees introduced by Bradford *et al.*^[17]. The observed constraint adherence reinforces the theoretical assertion that uncertainty-aware predictive models can prevent infeasible control actions and ensure closed-loop stability^[13-16]. Furthermore, the use of regularization and bounded-error loss functions during model training, as inspired by Haykin^[9] and Ljung^[8], contributed to greater robustness in dynamic environments.

Overall, the findings provide compelling evidence that ML-based MPC frameworks offer a practical balance among prediction accuracy, robustness, and computational efficiency. The GP-MPC approach excels in precision and uncertainty handling, RNN/LSTM-MPC offers efficient real-time performance, and ICNN/Koopman-MPC provides near-explicit optimization for fast industrial applications. These results align with the emerging paradigm of intelligent control systems, where data-driven methods complement classical control theory to enable adaptive and self-optimizing industrial operations^[2, 5, 11-19]. The present work thus substantiates the hypothesis that incorporating ML models with constrained predictive control yields a scalable and reliable framework for nonlinear process automation. Future directions include extending the framework to stochastic environments and hybrid physical-data-driven systems, further validating its industrial scalability and safety.

Conclusion

The integration of Machine Learning algorithms within Model Predictive Control (MPC) frameworks has demonstrated a significant advancement in controlling nonlinear industrial processes, establishing a foundation for intelligent and adaptive automation systems. The findings

from this study clearly indicate that data-driven predictive models such as Gaussian Processes (GP), Recurrent Neural Networks (RNNs), Long Short-Term Memory (LSTM) networks, and Input Convex Neural Networks (ICNNs) can substantially improve prediction accuracy, reduce transient deviations, and enhance the robustness of closed-loop performance compared to conventional linear and analytic nonlinear MPC systems. By capturing complex system nonlinearities and dynamic variations, these models offer predictive fidelity that traditional physics-based approaches often lack. The achieved improvements in stability, setpoint tracking, and computational efficiency confirm that incorporating Machine Learning into MPC enables real-time control with high precision and reliability, even in processes that exhibit strong nonlinearities and time-varying behavior. These outcomes validate the hypothesis that constrained and regularized learning models, when embedded within MPC, can maintain closed-loop stability while meeting the computational requirements of modern industrial environments.

In practical terms, these findings present multiple recommendations for real-world implementation. Industries relying on complex and nonlinear process operations—such as chemical, petrochemical, energy, and advanced manufacturing sectors—should gradually transition from static control architectures toward ML-augmented MPC frameworks. For large-scale plants, hybrid approaches combining first-principles and data-driven models can be adopted to balance interpretability with adaptability, ensuring that control decisions remain both explainable and robust under varying process conditions. For real-time deployment, it is advisable to employ computationally efficient structures like ICNN- or Koopman-based MPC, which provide fast optimization suitable for embedded industrial controllers. Process engineers should incorporate uncertainty estimation mechanisms within predictive models to safeguard against unanticipated disturbances and model drift, thus preserving operational safety. Furthermore, developing standardized pipelines for data acquisition, preprocessing, and model retraining is essential to maintain model accuracy and control reliability over time. Industries should also focus on establishing cross-functional teams that integrate process control expertise with Machine Learning proficiency, ensuring effective deployment and maintenance of these intelligent systems. Finally, incorporating continuous learning mechanisms within MPC—where models evolve through adaptive updates based on real-time data will further enhance decision-making precision and sustainability in industrial operations. By embracing these recommendations, organizations can leverage the synergy of control theory and Machine Learning to achieve superior process efficiency, energy optimization, and overall operational resilience in the era of smart manufacturing.

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