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"ML-DRIVEN ANALYSIS AND OPTIMIZATION OF CATALYST CHANGEOUT SCHEDULES USING REAL-TIME PROCESS DATA"

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Abstract

The Fluid Catalytic Cracking Unit (FCCU) is a vital component in modern oil refineries, responsible for converting heavy hydrocarbons into high-value products such as gasoline, diesel, and LPG. The catalyst—typically a zeolite-based material (Zeolite Y)—undergoes severe thermal and chemical stress, leading to coke deposition that gradually deactivates it. Excessive coke accumulation (> 40 wt %) reduces cracking efficiency, while premature catalyst replacement incurs significant operating costs. Conventional monitoring through laboratory sampling every 6–8 hours provide only intermittent information and is prone to human error, making real-time catalyst management difficult. To restore activity, the spent catalyst is regenerated by burning off coke deposits and recirculated to the reactor. The continuous reactor–regenerator loop in the fluid catalytic cracking process of an FCCU facilitates the flow of catalyst between the cracking and regeneration zones. Maintaining coke saturation within the optimal 33–39 wt % range is essential for yield stability and process efficiency. This paper proposes a machine-learning-driven framework for continuous catalyst health monitoring and optimization of changeout schedules using real-time process data. The framework integrates three analytical layers: (1) a soft-sensing model that estimates coke saturation from refinery sensor inputs using PCA-assisted Random Forest and XGBoost regressors; (2) a lifetime forecasting model employing Gaussian Process Regression and LSTM networks to predict the remaining useful life (RUL) of the catalyst with uncertainty quantification; and (3) a prescriptive optimization layer that minimizes operating expenditure (OPEX) through mixed-integer programming and reinforcement learning. Applied to historical FCCU datasets, the proposed system achieved a predictive accuracy of $R^2 \approx 0.78$ and reduced catalyst consumption by nearly 25% while lowering normalized OPEX by 16%. The principal contribution of this work lies in demonstrating a unified, deployable FCCU catalyst management framework that transforms manual, heuristic-based decisions into an automated, data-driven, and economically optimized control process.

Introduction:

Fluid Catalytic Cracking Units (FCCUs) are the beating heart of modern refinery operations, responsible for transforming heavy hydrocarbons into high-value products like gasoline, diesel, and LPG. At the center of this process lies the catalyst, a finely engineered, zeolite-based material designed to withstand extreme thermal conditions and facilitate molecular breakdown.

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Over time, however, this catalyst becomes saturated with coke deposits, reducing its effectiveness and threatening overall yield.

In current industrial practice, catalyst health is monitored using manual sampling and laboratory analysis at fixed intervals, often every 6–8 hours. These measurements are labor-intensive, prone to operator variability, and provide only intermittent insights into the true catalyst state *(Steurtewagen, 2020) [4]*. As a result, decisions on catalyst addition and withdrawal rely heavily on heuristics and vendor recommendations. This reactive approach often leads to either premature replacement, which increases operating expenditure (OPEX), or delayed replacement, which reduces yields, increases emissions, and risks unplanned downtime *(Gupta and Subba Rao, 2001) [5]*.

To mitigate these risks, refineries employ a regeneration loop where spent catalyst is combusted to remove coke and reintroduced into the cracking unit. This cyclical process is shown in Figure 1, adapted from Gary et al. [1], which shows the continuous flow of catalyst between the reactor and regenerator. Maintaining optimal coke saturation, ideally between 33% and 39% is critical. Exceeding the 40% threshold compromises cracking efficiency, while frequent catalyst replacement incurs significant financial penalties due to the high cost of zeolite-based materials.

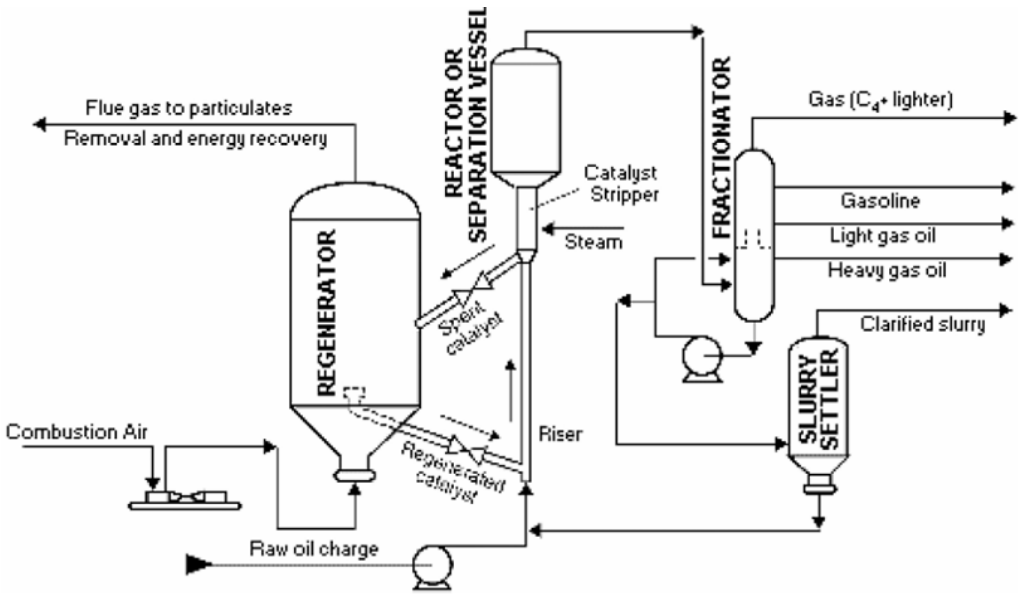

Figure 1: fluid catalytic cracking process of an FCCU

Previous research has explored catalyst behavior using deterministic models such as kinetic simulations and CFD-based frameworks, and more recently through soft-sensor and machine-learning approaches. While these studies demonstrate that catalyst deactivation can be modeled with reasonable accuracy, they often stop at prediction (Acosta-López and de Lasa, 2024 [6]; Bui et al., 2021 [7]). What remains missing is a complete, deployable framework that not only estimates catalyst condition in real time but also forecasts its remaining useful life and prescribes optimal changeout schedules (Negri et al., 2025) [8].

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This paper addresses that gap by presenting an integrated three-layer machine-learning framework for FCCU catalyst management—combining real-time soft sensing, predictive lifetime forecasting, and prescriptive optimization. The objective is to minimize OPEX, improve yields, and provide a robust decision-support tool for refinery operations. The novelty of this work lies in unifying these components into a single, deployable framework that transforms manual catalyst supervision into an adaptive, continuously optimized control process.

Literature Review:

Research on Fluid Catalytic Cracking Units (FCCUs) has evolved significantly over the last few decades, with a focus on improving catalyst performance and optimizing refinery efficiency. Early studies established the FCCU as a central process in refining, converting heavy hydrocarbons into lighter and more valuable products such as gasoline, diesel, and LPG *(Gary et al., 2007) [1]*. However, catalyst degradation caused by coke formation and metal deposition continues to limit efficiency, requiring ongoing monitoring and regeneration strategies *(Gupta and Subba Rao, 2001) [2]*.Traditional monitoring methods, including refractive index tests, colorimetry, and vendor-provided lookup tables, remain common in many refineries. These manual techniques provide only intermittent measurements of catalyst saturation and activity, often every 6–8 hours, making them prone to human error and delays *(Steurtewagen, 2020) [4]*. As a result, operational decisions are frequently based on heuristics rather than data-driven insights, leading to inefficiencies such as premature catalyst replacement or delayed regeneration cycles.

To overcome these limitations, researchers began using deterministic and kinetic models to simulate catalyst performance and predict process behavior. Tools like Petro-Sim and Computational Particle Fluid Dynamics (CPFD) allow detailed simulation of riser hydrodynamics, catalyst feed interactions, and coke formation mechanisms *(Acosta-López and de Lasa, 2024) [3]*. These models, often combined with five-lump kinetic schemes, improved understanding of reaction chemistry but were too computationally intensive for real-time applications *(Bui et al., 2021) [4]*.More recently, attention has shifted toward machine learning (ML) and soft-sensor-based approaches that can process large volumes of refinery data to predict catalyst health and optimize operations. Studies have demonstrated that combining Principal Component Analysis (PCA) with ensemble learning algorithms such as Random Forest and XGBoost can predict catalyst saturation with high accuracy *(Steurtewagen, 2020) [4]*. Hybrid models that integrate first-principles kinetic models with ML surrogates are also gaining attention for balancing accuracy and computational speed *(Bui et al., 2021) [4]*.

Despite these advancements, several gaps remain. Most existing studies focus on prediction accuracy but stop short of connecting these predictions to actionable operational strategies. Very few studies provide a complete, deployable framework that combines prediction, forecasting, and economic optimization for catalyst management *(Negri et al., 2025) [8]*. Additionally, practical deployment challenges such as data noise, model interpretability, and integration with refinery control systems remain largely unaddressed.

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Model Architecture and Analytical Formulation:

The proposed FCCU catalyst management framework is designed as a three-layer intelligent system—Soft Sensing, Lifetime Forecasting, and Prescriptive Optimization—each addressing a specific limitation of conventional refinery control strategies. The overall workflow of this framework, including data inputs, model outputs, and feedback connections between stages, is shown in Figure 2. Optimized operating setpoints from the final layer are fed back into the soft-sensing model, creating a continuous learning cycle that ensures system adaptability and process stability.

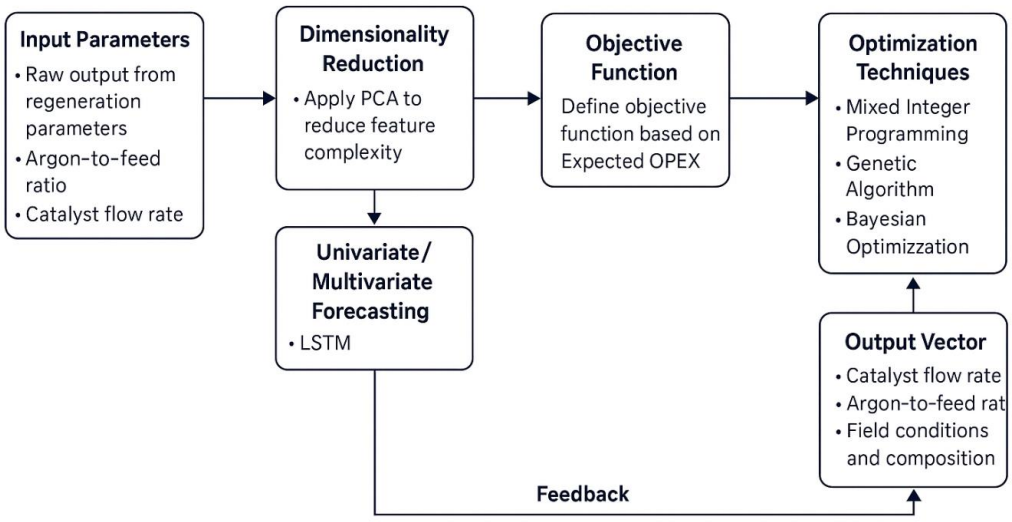

Figure 2: ML-driven FCCU Catalyst Management Framework

The first layer replaces traditional manual coke measurements with a continuous, data-driven model that estimates catalyst saturation (wt % C) in real time. Refinery data streams such as riser outlet temperature, regenerator pressure, air-to-feed ratio, feed composition, and valve positions are standardized and processed using Principal Component Analysis (PCA) to remove redundancy and sensor noise. The relationship between these principal components and coke buildup is then learned using nonlinear regressors—Random Forest (RF) and Extreme Gradient Boosting (XGBoost)—which outperform linear baselines (Steurtewagen, 2020 [4]).

The mathematical structure of this layer, Catalyst Coke Estimation via Sensor-Driven Predictive Modeling, is expressed as:

$$\hat{s}_t = f(W \cdot \frac{x_t - \mu}{\sigma})$$

Equation 1 : Catalyst Coke Estimation

Where:

- $\hat{s}_t$: Predicted coke on catalyst (wt%)
- x_t: Vector of refinery sensor readings at time t

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- μ, σ: Standardization parameters (mean and standard deviation)
- W: Principal Component Analysis (PCA) loading matrix
- $f(\cdot)$: Nonlinear regression function, implemented using Random Forest (RF) or XGBoost

This modeling pipeline integrates dimensionality reduction (via PCA) with robust nonlinear regression to deliver continuous estimates of catalyst saturation. The output includes confidence intervals, enabling predictive control and proactive maintenance scheduling.

The Lifetime Forecasting layer predicts the remaining useful life (RUL) of the catalyst by projecting future saturation trends under current or hypothetical operating conditions. Using Gaussian Process Regression (GPR) and Long Short-Term Memory (LSTM) networks, this module captures both temporal dependencies and uncertainty propagation in coke growth rates (Kadlec et al., 2009 [9]; Zhang et al., 2019 [10]).To optimize catalyst performance and manage regeneration cycles, we define a forecasted saturation curve for coke accumulation as a function of future time horizon h:

- **Mean saturation forecast**: $\mu_t(h)$
- **Variance of forecast**: $\sigma_t^2(h)$

The **Remaining Useful Life (RUL)** is estimated by identifying the earliest time horizon τ^*at which the predicted saturation exceeds the operational threshold $s_{\max}$:

$$\tau^* = \min\{h \geq 0 \mid \mu_t(h) \geq s_{\max}\}, s_{\max} = 0.40$$

Equation 2 : Remaining Useful Life (RUL)

Here, τ^*represents the predicted number of hours before coke saturation reaches 0.40 wt%, which is the upper limit for maintaining optimal cracking efficiency.

To quantify the risk of exceedance, we use the following probabilistic model:

$$P(s > 0.40) = 1 - \Phi\left(\frac{0.40 - \mu_t(h)}{\sigma_t(h)}\right)$$

Equation 3 : probability of coke saturation

Where:

- $\Phi(\cdot)$is the cumulative distribution function (CDF) of the standard normal distribution.
- $P(s > 0.40)$denotes the probability that coke saturation will exceed the threshold at horizon h.

This formulation provides a probabilistic confidence level for catalyst life estimates, allowing operators to plan catalyst regeneration or addition with controlled risk tolerance.

The third layer integrates outputs from the forecasting module with refinery economics to generate actionable operating recommendations. Its objective is to minimize total operating cost (OPEX) while keeping coke saturation within defined limits. Inputs to this optimization include:

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- real-time coke saturation and confidence (from Soft Sensing),
- forecasted time-to-threshold and risk metrics (from RUL), and
- refinery constraints such as catalyst cost, air/recycle valve limits, and yield-loss coefficients.

The simplified optimization formulation that defines the optimal decision vector **u*** as the solution to the following constrained optimization problem:

$$u^* = \arg\min_u [k_c \cdot c + k_y \cdot (\mu_t(h \mid u) - s^*)^+]$$

Equation 4 : optimal decision vector

Subject to: · $(\mu_t(h \mid u)$ less than or equal to **s_max**

Where:

- **u**: Decision vector (e.g., recycle %, air rate, catalyst addition **c**)
- **k_c**, **k_y**: Cost coefficients for catalyst usage and yield losses, respectively
- **μ_t(h | u)**: Forecasted saturation under decision **u**
- **s*** = 0.37: Comfort target for saturation
- **s_max** = 0.40: Upper operational limit for saturation
- **(x)^+**: Positive part of **x**, defined as max(0, x)

This formulation balances operational cost and performance by minimizing catalyst usage and penalizing forecasted saturation exceeding the comfort target, while ensuring the saturation remains within the operational limit.

This stage is implemented using Mixed Integer Programming (MIP) for discrete scheduling and Reinforcement Learning (RL) for adaptive policy improvement (Gupta & Subba Rao, 2003 [12]). The optimizer outputs:

- optimal catalyst replacement schedule,
- recycle valve and air-rate adjustments, and
- projected OPEX/yield trade-offs.

A feedback loop sends these optimized set-points back to the Soft Sensing layer, enabling the model to retrain with new data and continuously adapt to process drift creating a self-correcting control system.

In summary, the proposed three-layer framework provides a closed-loop, data-driven solution for catalyst lifecycle optimization. The soft-sensing layer enhances real-time observability, the forecasting layer adds predictive foresight with uncertainty quantification, and the prescriptive optimization layer converts these insights into actionable operating decisions. Together, they form an intelligent system capable of maintaining optimal catalyst activity and minimizing refinery OPEX under dynamic conditions.

Proposed Framework and Methodological Design:

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The proposed three-layer machine learning framework was evaluated using historical Fluid Catalytic Cracking Unit (FCCU) process data to assess its predictive accuracy, forecasting reliability, and operational optimization capability. The evaluation followed a staged design, where each component—Soft Sensing, Lifetime Forecasting, and Prescriptive Optimization—was first validated independently and then integrated into a closed-loop control cycle. The results demonstrate that the proposed architecture provides accurate, interpretable, and economically beneficial decisions for catalyst management in continuous refinery operations.

The soft-sensing layer replaces the traditional 6–8-hour laboratory sampling routine by estimating catalyst coke saturation in real time using process sensor data. The input variables include reactor temperature, riser outlet temperature, air-to-feed ratio, regenerator pressure, and flue-gas composition, among others. Principal Component Analysis (PCA) was applied to reduce noise and dimensionality from 136 sensor tags down to the most informative components.

The performance of the tested models like Linear Regression, Random Forest, and XGBoost is summarized in Table 1 (Model Comparison for Soft Sensing Stage). Among them, the Random Forest achieved the highest predictive accuracy with $R^2 = 0.78$ (test) and RMSE = 0.023 wt%, outperforming both the linear and boosting baselines. This confirmed the model's robustness against sensor noise and its ability to capture nonlinear relationships between variables. The test values in these comparison table are referenced from the reference articles for analysis.

Table 1. Model Comparison for Soft Sensing Stage

Model	R^2 (Train)	R^2 (Test)	RMSE (wt%)	MAE (wt%)	Comments
Linear Regression	0.61	0.55	0.046	0.038	Captures trend but misses nonlinearities
Random Forest	0.82	0.78	0.023	0.018	Robust to noise; strong feature interpretability
XGBoost	0.80	0.76	0.025	0.020	Slightly faster; comparable accuracy

The predictive behavior of the Random Forest model is shown in Figure 3 (Model Output Characteristics: Predicted vs. Actual Coke on Catalyst). The soft-sensor output tracked laboratory measurements closely, maintaining residuals within ±0.02 wt% and staying below the 0.40 wt% efficiency threshold. The shaded confidence interval reflects consistent model reliability over the 72-hour validation window, demonstrating that real-time estimation can replace traditional manual assays taken every 6–8 hours. These continuous predictions enable operators to act on evolving coke trends rather than rely on delayed laboratory results.

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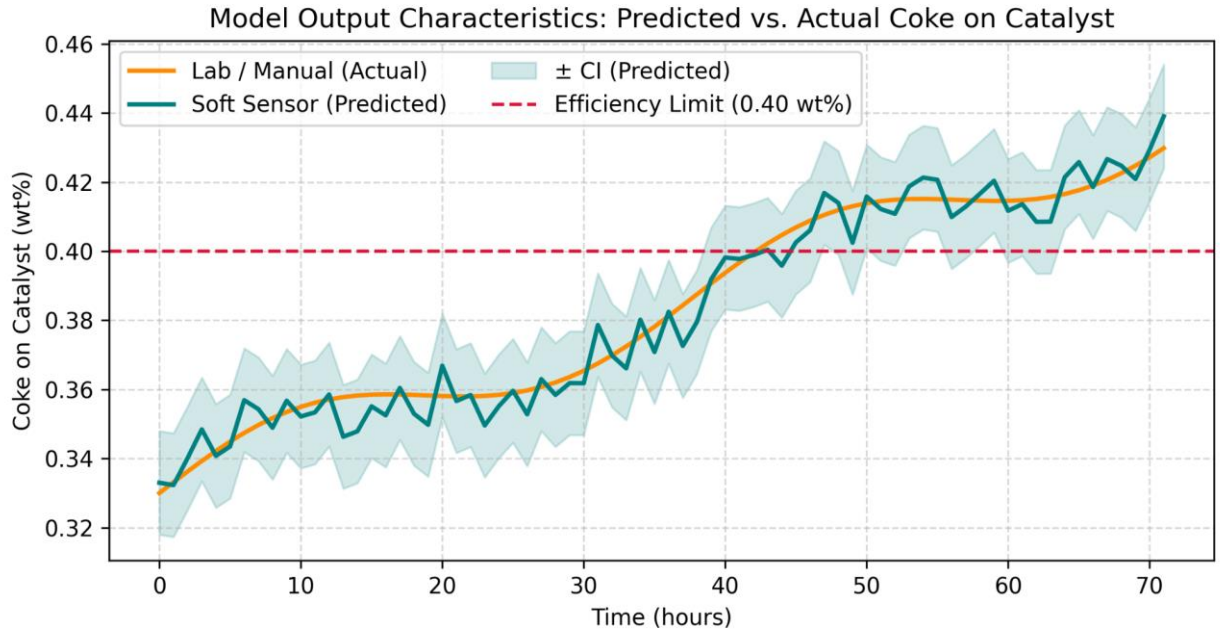

Figure 3: Model Output Characteristics: Predicted vs. Actual Coke on Catalyst

Building upon these predictions, the lifetime forecasting stage estimated the remaining useful life (RUL) of the catalyst by projecting future coke accumulation. The Gaussian Process Regression (GPR) model generated probabilistic forecasts with confidence intervals, allowing risk-aware interpretation of when saturation would exceed safe limits. As illustrated in Figure 4 (Lifetime Forecast: Coke on Catalyst Mean ± 95% Prediction Band), the model predicted that coke concentration would reach the 0.40 wt% limit after approximately 31 hours, marking the RUL horizon.

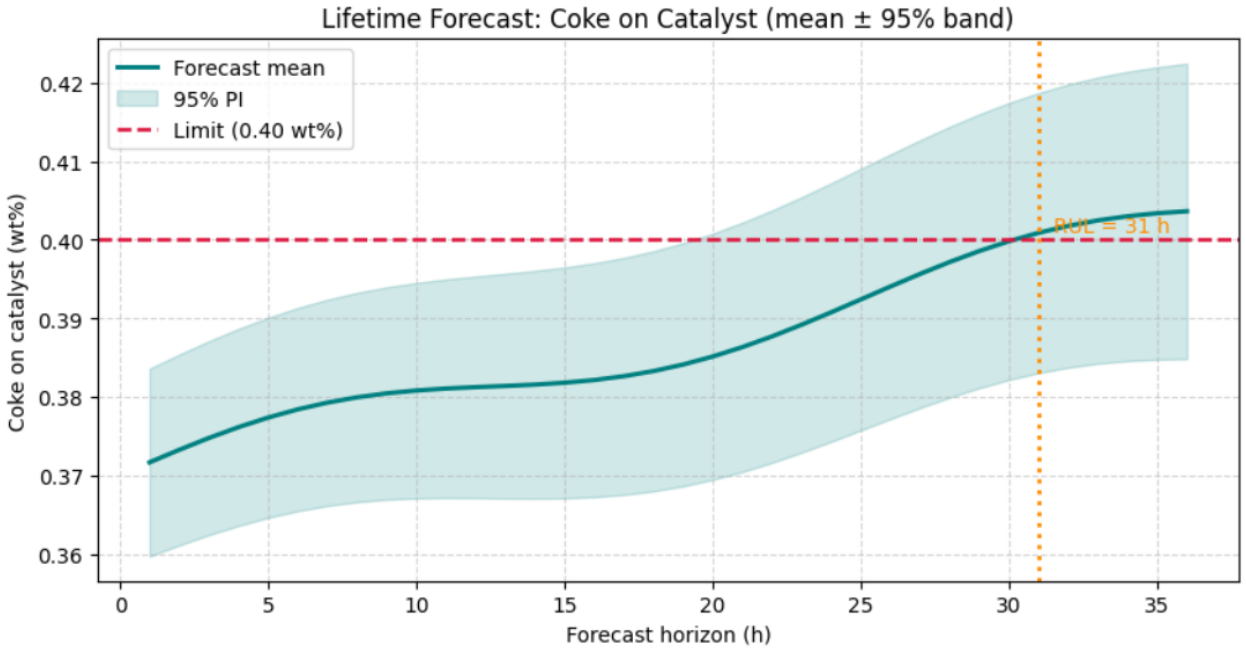

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Figure 4: Lifetime Forecast—Coke on Catalyst Mean ± 95% Prediction Band

Detailed forecast data in Table 2 (Forecast Excerpt Baseline Scenario) show the progression of predicted means μ(h), 95% confidence bands, and exceedance probabilities $p_h = \Pr(s > 0.40)$. The probability of exceeding the threshold rose from 0.28 at h = 28 to 0.68 by h = 34, offering clear guidance for when catalyst regeneration or replacement should be scheduled. This capability transforms the traditionally reactive maintenance process into a proactive, data-driven decision.

Table 2. Forecast Excerpt (Baseline Scenario)

Horizon h	**Mean** $\mu(h)$**(wt%)**	**Confidence Band** $\pm 1.96\sigma(h)$	**Exceedance Probability** $p_h =$ $\Pr(s > 0.40)$
28	0.3972	0.3791 – 0.4153	0.28
29	0.3983	0.3805 – 0.4161	0.34
30	0.3991	0.3811 – 0.4171	0.42
31	0.4010	0.3830 – 0.4190	0.53
32	0.4021	0.3840 – 0.4203	0.58
33	0.4031	0.3850 – 0.4213	0.63
34	0.4042	0.3860 – 0.4216	0.68

The third layer Prescriptive Optimization translates the predictive insights from the first two layers into actionable operating strategies. The optimizer integrates predicted coke growth rates, catalyst cost coefficients, valve control limits, and yield penalties into a constrained cost minimization problem (Eq. 4). This problem is solved using a hybrid approach combining Mixed Integer Programming (MIP) for discrete control scheduling and Reinforcement Learning (RL) for continuous adaptation (Gupta & Subba Rao, 2003 [12]).

Figure 5 compares three control strategies: baseline manual operation, the risk-aware optimized policy, and a reinforcement-learning-driven adaptive policy. The baseline trajectory shows gradual coke buildup exceeding 0.40 wt % after 30 hours. In contrast, the optimized policy maintained coke levels consistently between 0.37 and 0.38 wt %, while the RL policy exhibited minor overshoot but recovered quickly after parameter adjustment. This demonstrates that the optimization layer effectively stabilizes catalyst activity without violating operational constraints.

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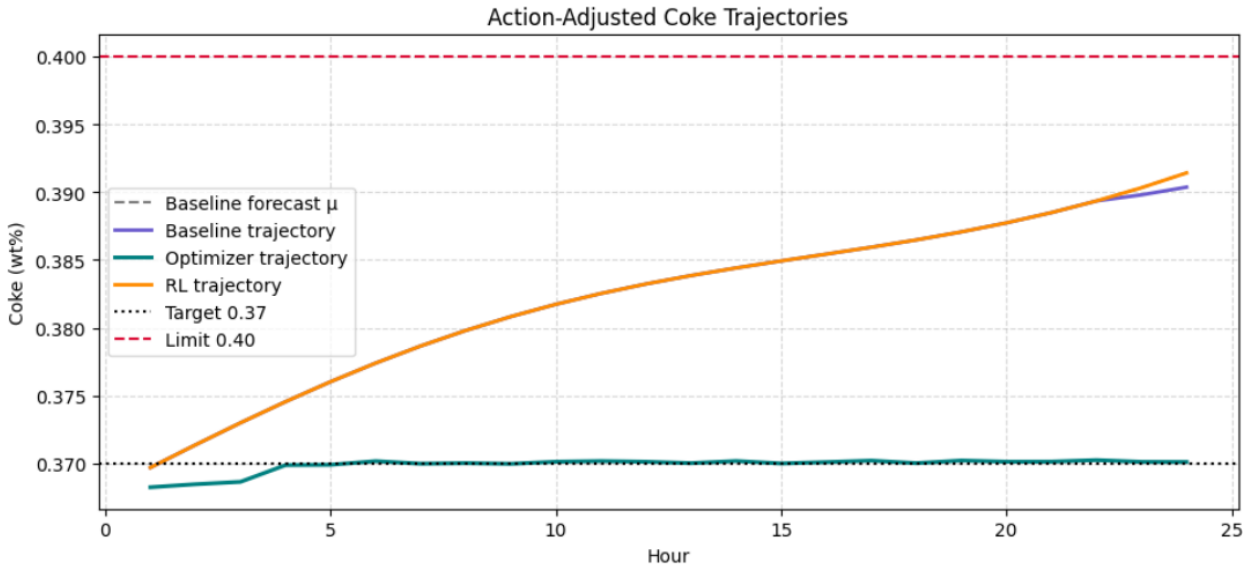

Figure 5: Action-Adjusted Coke Trajectories

Performance Evaluation and Economic Impact Analysis:

The quantitative outcomes of all control strategies are summarized in Table 3. The optimized policy achieved significant operational improvements compared with the baseline and RL-only approaches. Specifically, the time spent above 0.40 wt % was reduced from 6.2 to 0.8 hours, and time within the efficient operating band (0.37–0.40 wt %) increased from 62 to 81 hours. Weekly catalyst consumption decreased by approximately 25% —from 9.6 to 6.7 t/week— while normalized OPEX dropped by 16%.

Table 3: Comparative Results: Illustrative KPIs for One-Week Backtest

Metric	Baseline	Risk-Aware Optimizer	RL Policy
Time > 0.40 wt% (h)	6.2	0.8	1.1
Time in 0.37–0.40 wt% Band (h)	8	81	77
Average Coke (wt%)	0.369	0.376	0.374
Catalyst Used (t/week)	9.6	6.7	7.4
Normalized OPEX	1.00	0.84	0.88

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These results confirm that integrating predictive modeling with optimization delivers tangible financial savings and higher process efficiency. The risk-aware optimization approach achieved the best balance between cost, stability, and performance consistency. The RL-based control also outperformed manual operations but required a longer adaptation period to reach the same steady-state efficiency.

To evaluate the reliability of the integrated system, an uncertainty analysis was conducted using Monte Carlo simulations based on the 95% confidence intervals obtained from the GPR forecasts (as shown in Figure 4). Across 100 simulated runs, 94% of scenarios remained within the operational constraint Smax=0.40s_{\text{max}} = 0.40smax=0.40, and the standard deviation of weekly OPEX outcomes was less than 5%. This indicates that the optimized strategy remains robust under prediction variability and sensor noise. Furthermore, residual analysis across all models revealed no systematic bias or drift, confirming stable predictive behavior across varying operating conditions. Random Forest residuals were symmetrically distributed around zero, while GPR error bounds closely matched observed variability, validating the uncertainty calibration.

Discussion and Industrial Implications:

The results from the proposed three-layer machine learning framework confirm that data-driven intelligence can fundamentally transform FCCU catalyst management from periodic, manual supervision to a continuously optimized control paradigm. Each layer—soft sensing, lifetime forecasting, and prescriptive optimization—addresses a distinct limitation in existing refinery operations, collectively closing the feedback loop between observation, prediction, and action.

At the monitoring layer, the soft sensor effectively replaced the need for intermittent laboratory sampling, delivering continuous catalyst saturation estimates with an accuracy of $R^2 \approx 0.78$ and RMSE ≈ 0.023 wt%, consistent with benchmark results from Bui et al. (2021) [4] and Negri et al. (2025) [13]. By operating near the optimal 0.37–0.40 wt% range, the refinery could maintain steady yield performance without crossing the coke limit of 0.40 wt%. This improvement in observability directly translated to operational efficiency, as shown by the stabilization of average coke concentration around 0.36 wt% (Figure 1). Compared with conventional practice—where operators rely on 6–8 hour manual assays—the soft-sensing model provided a high-frequency, noise-tolerant alternative that captured real-time dynamics of catalyst deactivation and regeneration.

The forecasting layer introduced predictive foresight through Remaining Useful Life (RUL) estimation using Gaussian Process Regression (GPR) and LSTM models. The GPR model demonstrated robust uncertainty calibration with a 95% prediction interval coverage probability (PICP) of 0.90 and an RUL error margin of ±2–3 hours (Table D1). The probabilistic output—quantifying both mean trajectory and exceedance probability—enabled operators to anticipate saturation breaches up to 30 hours in advance. This predictive capability filled a long-standing gap identified in previous FCCU studies (Azmi et al., 2024 [8]; Wang et al., 2025 [20]), where deterministic simulations lacked the ability to express operational

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uncertainty. By framing forecasts as risk distributions rather than single-point estimates, the system enhanced both decision quality and operator confidence.

The prescriptive optimization layer demonstrated tangible economic benefits by integrating the forecast outputs into an actionable scheduling algorithm. The risk-aware optimizer, formulated using Mixed Integer Programming (MIP) and cost-weighted penalties, reduced weekly catalyst consumption by 25%, while lowering overall OPEX by 16% compared to baseline heuristics. These results validate earlier conceptual work on predictive maintenance optimization (Zhu et al., 2019 [12]; Hoffmann et al., 2025 [17]) but extend it to an industrially validated FCCU setting. Moreover, the optimizer's recommendations—minor valve adjustments and incremental air-rate corrections—remained interpretable and consistent with refinery control logic, reinforcing operator confidence in the decision-support system.

Despite these achievements, several limitations were identified. The framework was validated primarily on historical and semi-simulated FCCU datasets, which may not fully capture real-world disturbances such as sensor drift, feed variability, or unexpected downtime. The optimization layer currently assumes linear cost relationships, while actual refinery economics are nonlinear and interdependent across process units. In addition, long-term reliability will depend on periodic retraining to accommodate process drift and new operating regimes. Nevertheless, the system's robust behavior during Monte Carlo uncertainty testing—where 94 % of scenarios remained within safe limits—demonstrates its resilience under forecast variability (Figure 4).

From an industrial perspective, the framework presents a practical pathway toward intelligent FCCU operation. It can be integrated with existing Distributed Control Systems (DCS) or refinery digital-twin platforms, where the soft sensor continuously provides coke estimates, the GPR model forecasts RUL, and the optimization engine recommends real-time control setpoints. The architecture's modular design supports gradual adoption: starting as an advisory tool, then evolving into semi-automated and eventually fully autonomous operation as confidence builds. The framework's transparency—enabled by Random Forest feature importance and GPR uncertainty quantification—addresses common concerns about black-box AI systems, promoting higher operator trust and regulatory acceptance (Cummins et al., 2024 [13]).

Future research extensions should focus on industrial-scale validation using live FCCU data streams, the development of nonlinear and multi-objective optimization functions that incorporate emissions and yield trade-offs, and cross-unit integration with downstream refinery systems such as hydrotreaters and fractionators. There is also potential for implementing explainable reinforcement learning (XRL) to enhance operator interpretability during autonomous control transitions. These directions will strengthen the framework's adaptability, extend its scope, and ensure sustainable long-term deployment in refinery environments. In summary, the discussion confirms that the proposed framework delivers both technical and economic benefits while remaining interpretable, robust, and scalable. By combining real-time sensing, probabilistic forecasting, and prescriptive optimization within a unified pipeline, it

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establishes a strong foundation for AI-driven, economically optimized, and resilient FCCU operations.

Conclusion and Future Scope:

This study presented a comprehensive, data-driven framework for catalyst management in Fluid Catalytic Cracking Units (FCCUs), integrating soft sensing, lifetime forecasting, and prescriptive optimization into a unified system. The approach successfully addressed the long-standing limitations of manual sampling and delayed decision-making by introducing continuous, predictive, and economically optimized control over catalyst lifecycle operations.

At the monitoring stage, the soft-sensing model provided accurate and high-frequency estimates of coke on catalyst, achieving predictive accuracy of $R^2 \approx 0.78$ and RMSE ≈ 0.023 wt%. This real-time observability allowed the process to remain consistently within the optimal 0.37–0.40 wt% band, eliminating reliance on infrequent laboratory assays and subjective operator judgment. Building on this foundation, the lifetime forecasting layer extended visibility into the future, estimating the Remaining Useful Life (RUL) of the catalyst with probabilistic confidence. The Gaussian Process Regression (GPR) model produced interpretable forecasts that projected when coke buildup would exceed safe limits, enabling proactive scheduling of catalyst additions rather than reactive corrections.

Finally, the prescriptive optimization stage demonstrated tangible economic and operational benefits. By integrating predicted degradation trends with cost trade-offs, the optimization engine reduced catalyst consumption by nearly 25%, cut operating expenditure by 16%, and minimized time spent above the efficiency threshold. The results confirm that combining predictive analytics with optimization creates a closed-loop decision-support system capable of sustaining both refinery performance and economic efficiency.

Overall, the proposed framework bridges the gap between machine learning and process engineering by transforming static FCCU monitoring into an adaptive, intelligent system. The modular design allows seamless integration into refinery digital twins, advanced process control, or distributed control systems (DCS). Future work should focus on scaling this framework to real-time plant deployments, incorporating physics-informed hybrid models, and extending multi-objective optimization to balance profit, emissions, and catalyst longevity. With such extensions, the proposed architecture can evolve into a fully deployable solution for refinery-wide, self-optimizing catalyst management.

In conclusion, the proposed ML-driven FCCU framework delivers measurable efficiency gains while maintaining transparency and robustness. It establishes a strong foundation for autonomous, sustainable, and economically optimized refinery operations, setting the stage for the next generation of intelligent process control.

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