

# Predictive Analytics for Reducing Title V Deviations in Chemical Manufacturing

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## ABSTRACT:

The Title V operating permits require chemicals manufacturing facilities to comply with stringent air emissions limits, monitoring, recordkeeping, and reporting provisions. Despite robust Environmental Management Systems (EMS), deviations continue to occur due to manual monitoring limitations, complex regulatory obligations, and the variability of industrial processes. This study proposes a predictive analytics framework designed to anticipate Title V deviations before they occur. Using statistical modeling, machine learning (ML), historical deviation data, continuous emissions monitoring system (CEMS) inputs, and operational parameters, the framework estimates the probability of future deviations and identifies key drivers. Case simulations demonstrate that predictive modeling can reduce deviations by 30–55% by enabling proactive operational adjustments, improved recordkeeping, and targeted corrective actions. The approach is designed to complement existing facility-specific permit conditions. Results show that predictive analytics can shift air compliance programs from reactive detection to proactive prevention, improving compliance consistency across multi-unit chemical operations.

**Keywords:** Title V, predictive analytics, emissions compliance, machine learning, environmental management, air permitting, EPA, data-driven compliance

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## I. INTRODUCTION

The chemical manufacturing facilities, classified as “major source”, regulated under the U.S. Clean Air Act (CAA) operate under complex, facility-wide operating permits known as Title V permits. These permits incorporate federally enforceable air emissions control requirements for a source, including federal, state rules, and site-specific permit conditions. This consolidation is intended to improve compliance clarity and transparency but, in practice, creates a highly intricate regulatory landscape for large chemical plants.

Under Title V, a major chemical source must demonstrate continuous compliance with all applicable requirements, which often include:

- a) New Source Performance Standards (NSPS) under 40 CFR Part 60, such as subparts for process heaters, boilers, storage tanks, flares, and specific chemical production units. These standards generally impose emission limits, monitoring methods, testing, and recordkeeping for criteria pollutants and sometimes hazardous air pollutants.
- b) National Emission Standards for Hazardous Air Pollutants (NESHAP) under 40 CFR Part 63, which set technology-based standards for hazardous air pollutants (HAPs). For chemical manufacturing, this often includes maximum achievable control technology (MACT) standards for chemical production, miscellaneous organic NESHAP (MON), refinery operations, and other HAP-intensive processes.
- c) State Implementation Plans (SIPs), which incorporate state-specific rules such as volatile organic compound (VOC) control rules, NO<sub>x</sub> reasonable available control technology (RACT), seasonal ozone strategies, and other regional requirements that apply in addition to federal NSPS/NESHAP.
- d) Leak Detection and Repair (LDAR) requirements, which may arise from MACT standards, NSPS, consent decrees, or state programs. These are designed to detect fugitive emissions from valves, pumps, connectors, and other components.

e) CEMS and parametric monitoring, which provide continuous records of key pollutants (e.g., NO<sub>x</sub>, SO<sub>2</sub>, CO, VOCs) and surrogates (e.g., combustion temperature, oxygen levels, pressure drops). These monitoring systems are critical for demonstrating compliance with short-term and long-term limits, but they also introduce complex data management and QA/QC requirements.

Title V permits integrate all of these moving parts into a single compliance framework; deviations can arise from multiple failure modes. In practice, Title V deviations at chemical manufacturing facilities frequently result from:

- a) **Monitoring failures:** CEMS or CMS downtime, calibration drift, data acquisition system failures, missing averages, or invalidated data periods that are not addressed within regulatory timeframes.
- b) **Operational exceedances:** Short-term or long-term exceedances of emission limits or surrogate parameters, such as minimum combustion temperature for a thermal oxidizer, maximum flare tip velocity, excessive boiler load leading to NO<sub>x</sub> exceedances, or operating outside allowable ranges specified in MACT or NSPS requirements.
- c) **Recordkeeping gaps:** Missing logs, incomplete operator entries, lack of documentation of control device setpoints, or missing certification of inspections for storage tanks, LDAR components, or BWON-affected equipment.
- d) **Late or inaccurate reporting:** Semiannual or annual compliance reports, deviation reports, excess emission reports, and performance test submittals that are not filed on time, or that fail to fully disclose deviations, root causes, and corrective actions.
- e) **Equipment malfunction or maintenance lapses:** Failures of control devices, dampers, monitoring instruments, or process equipment that are not promptly identified or corrected, leading to unpermitted emissions or extended operation outside approved parameters.
- f) **Permit condition complexity across multiple units:** Large Title V permits often contain hundreds or thousands of conditions covering dozens of emission units, each with different averaging times, monitoring methods, and reporting triggers. This complexity increases the risk of human error, inconsistent interpretation, and gaps in task execution, especially in multi-site or multi-business-unit organizations.

Traditional compliance auditing and deviation management are inherently reactive: issues are discovered after the fact through periodic internal audits, external agency inspections, or retrospective review of monitoring data and reports. By the time a deviation is identified, the noncompliance period may already have occurred, potentially for weeks or months, exposing the facility to enforcement risk, penalties, and reputational harm.

Predictive analytics offers a fundamentally different paradigm. By leveraging historical deviation data, CEMS and parametric time series, maintenance records, and operational data, statistical and machine-learning models can be trained to:

- a) Estimate the probability of future deviations under current or upcoming operating conditions.
- b) Identify leading indicators and root cause patterns associated with deviations (e.g., specific ranges of load, temperature drift, or increasing CEMS variability).
- c) Generate early warning alerts to operators and environmental staff, enabling corrective action before a limit is exceeded or required monitoring is lost.
- d) Support risk-based prioritization of inspections, maintenance, and management attention across units, permits, or sites.

In this way, predictive analytics enables a shift from “after-the-fact” compliance confirmation to proactive risk management, aligning with modern concepts of digital environmental management systems and continuous improvement in Title V compliance performance (Dias B.L., 2020).

## II. BACKGROUND AND LITERATURE REVIEW

Historically, environmental compliance systems have depended on manual recordkeeping, retrospective audits, and periodic reviews of emissions and operational data. These traditional approaches, while foundational, are increasingly insufficient for addressing the highly dynamic and tightly regulated nature of modern chemical processes. Over the last

decade, a growing body of literature has demonstrated the potential of machine learning (ML), statistical modeling, and automated data analysis to enhance environmental performance and reduce regulatory risk.

### **2.1 ML-Based Anomaly Detection for CEMS and Emissions Monitoring**

CEMS generate large high-frequency datasets that are ideal for anomaly detection and predictive modeling. Machine learning algorithms, particularly Random Forests and neural networks, can effectively detect abnormal emission patterns indicative of potential exceedances, calibration drift, or instrument malfunction [1]. Recent research on supervised and unsupervised models demonstrates that deviations from expected operational behavior could be detected before they trigger permit violations [2]. Such approaches are highly relevant to Title V compliance, where CEMS downtime or invalid data periods often constitute deviations.

Other studies have reinforced the potential of ML in emissions monitoring, including time-series forecasting methods that predict pollutant concentrations based on operational conditions, fuel variability, and combustion efficiency metrics [3]. These advancements provide a foundation for forecasting Title V deviations related to short-term emission limits and parametric requirements.

### **2.2 Predictive LDAR Scheduling and Fugitive Emissions Reduction**

Leak Detection and Repair (LDAR) programs are required under numerous NSPS and MACT standards and are prominent contributors to Title V deviation reporting. Traditionally, LDAR screening frequencies are fixed by regulation. Subsequent industry case studies showed how predictive LDAR tools can prioritize “high-risk” components, such as valves with repeated leaks or pumps operating under variable load, allowing facilities to allocate labor more efficiently while reducing emissions and regulatory risk. These insights translate directly to predicting deviations tied to LDAR monitoring failures, delayed repair timelines, or missed inspections.

### **2.3 Predictive Maintenance for Pollution Control Equipment**

Pollution control equipment (e.g., thermal oxidizers, scrubbers, flares, selective catalytic reduction units) plays a central role in maintaining compliance with MACT, NSPS, and Title V permit limits. Recent research demonstrated that integrating IoT sensors with predictive maintenance algorithms can identify early signs of equipment degradation, such as temperature drift, catalyst fouling, pressure drop anomalies, or burner instability [4].

Predictive maintenance has been shown to reduce unplanned downtime by 40–60% in comparable industries, which directly reduces the likelihood of emissions exceedances and monitoring deviations. As many Title V deviations are linked to equipment malfunction or maintenance lapses, extending predictive modeling to control devices is a highly relevant capability.

## **III. METHODOLOGY**

The proposed methodology for developing a predictive analytics system to reduce Title V deviations in chemical manufacturing includes four core modules, each addressing a key component of compliance risk evaluation:

1. Data Integration
2. Predictive Modeling
3. Deviation Risk Scoring
4. Operational Response & Control Strategies

These modules function as a continuous loop, forming a proactive, data-driven environmental compliance management system. The methodology is designed to be technology-agnostic but compatible with commonly used industrial platforms such as OSIsoft PI, AspenTech, Ignition SCADA, Honeywell Uniformance, and modern cloud analytics ecosystems.

### 3.1 Data Integration

Effective predictive modeling relies on the ability to capture, standardize, and process large volumes of heterogeneous data originating from environmental, operational, and regulatory systems. Chemical manufacturing facilities typically generate millions of data points per day, but these datasets are siloed across various systems, CEMS, SCADA, LIMS, CMMS, DCS, regulatory reporting software, and manual logs. The data integration phase consolidates these diverse data streams into a single, structured format suitable for advanced analytics.

Table 1. Data Categories and their Importance for Predictive Title V compliance

Data Category	Example Inputs	Importance for Predictive Modeling
(A)Operational Data	Reactor temperature, Thermal oxidizer combustion chamber temperature, Boiler steam load, Pressure and flow rates, Oxygen content	Operational variability is a major early indicator of emissions instability. Many Title V limits rely on surrogate parameters (e.g., minimum temperature requirements for MACT), making these variables essential for predicting exceedances.
(B)Emissions Data (CEMS/CPMS)	Nox, CO, SO <sub>2</sub> , VOCs, HAPs (benzene, toluene, formaldehyde), O <sub>2</sub> diluent corrections	CEMS/CPMS data directly reflects regulatory compliance status. Trends and volatility signal potential exceedances, rolling-average failures (1-hr, 3-hr, 24-hr), calibration drift, or invalid data periods—common causes of Title V deviations.
(C) Maintenance Data	Work orders, Preventive maintenance schedules, Equipment failure logs, Downtime records	Maintenance lapses strongly correlate with deviations. Predicting issues like scrubber failures, oxidizer burner fouling, or pump outages helps avoid VOC spikes, parametric upsets, and CEMS downtime.
(D) Environmental Compliance Data	Historical deviation logs (≥5 years), LDAR monitoring/repair frequency, Compliance task completion history	Provides ground truth for model training. Helps identify systemic issues (e.g., persistent unit problems, operator error, repeat LDAR leaks). Essential for supervised machine learning classification.
(E) Permit Data	Emission limits (mass, concentration), Surrogate parameter thresholds, Averaging periods (rolling 1-hr, 3-hr, 24-hr, block), MACT/NSPS statistical limits	Defines the regulatory boundaries that predictive models must forecast. Determines when predicted values constitute a potential deviation.
(F) Weather Data	Ambient temperature, Humidity, Wind speed/direction	Weather affects combustion efficiency, flare performance, evaporative emissions, and fenceline HAP readings. Meteorological variability often correlates with emission spikes or abnormal dispersion patterns.

#### 3.1.2 Data Warehouse Architecture

All datasets are cleaned, validated, and merged using a unified data warehouse consisting of:

- ETL pipelines (Extract-Transform-Load)
- Time-aligned data indexing
- Feature engineering scripts
- Handling of missing/unreliable data
- Outlier detection and normalization

Some examples of engineered features include rolling averages (1-hr, 3-hr, 24-hr), rate-of-change features ( $\Delta$ temp/min,  $\Delta$ load/hr), variance and standard deviation windows, control device stability indices and ‘Stress indicators’ (e.g.,

deviation precursors). The output of this step is a machine-learning-ready dataset that captures both short-term operational dynamics and long-term compliance behavior.

#### IV. PREDICTIVE MODELING FRAMEWORK

Title V deviations arise from complex interactions among operational conditions, emissions behavior, equipment performance, weather influences, and human/administrative processes. Because of this complexity, the predictive framework integrates three complementary modeling families:

1. Statistical regression models: for baseline explainability and linear risk estimation
2. Machine learning classification models: for nonlinear, multi-variable interactions
3. Time-series forecasting models (LSTM): for forecasting future emission and parametric trends

This combination allows the system to capture simple trends, nonlinear effects, and temporal dependencies in a unified predictive architecture.

##### 4.1 Statistical Models

Statistical models provide an interpretable foundation for deviation prediction. They are often preferred by regulatory agencies and internal stakeholders because they allow clear attribution of causal factors. Logistic regression [5] is used to estimate the probability of a Title V deviation over the next operational window (e.g., 15 minutes, 1 hour, or 24 hours). This method is appropriate when the outcome is binary: deviation vs. no deviation. Equation (1) represents this model:

$$p_d = P(\text{Deviation at time } t + 1) \tag{1}$$

The logistic model is:

$$\text{logit}(p_d) = \beta_0 + \beta_1 T + \beta_2 F + \beta_3 L + \beta_4 C_{\text{var}} + \beta_5 D_{\text{past}} \tag{2}$$

Where:

$\beta_i$	Coefficient	Parametric influence on deviation likelihood
$T$	Temperature	Surrogate for MACT/NSPS limits on thermal oxidizers, boilers
$F$	Flow	Impacts emissions dispersion, combustion efficiency
$L$	Equipment load (%)	High load correlates with NO <sub>x</sub> , CO, VOC deviations
$C_{\text{var}}$	CEMS variability	Measures signal instability; indicator of calibration drift
$D_{\text{past}}$	Past deviations	Captures historical patterns; deviations cluster in time

The deviation probability output can be represented by the following equation

$$p_d = \frac{1}{1 + e^{-\text{logit}(p_d)}} \tag{3}$$

The model produces a quantitative risk score between 0 and 1, enabling:

- Pre-emptive operator alerts
- Automatic escalation via EMS dashboards
- Risk-based prioritization of investigations

Some of the advantages include high transparency and interpretability, assistance with regulatory communication and fast computation for real-time applications. However, limitations such as assumption of linear relationships and inability to capture complex nonlinear behavior in emissions systems pose challenges to this approach.

##### 4.2 Random Forest Feature Importance Equation

Machine learning develops “feature importance” scores to determine which variables most strongly influence deviations [6].

$$I(f_k) = \sum_{t \in T_k} \frac{N_t}{N} \Delta G_t \quad (4)$$

Where:

$T_k$	Set of all decision-tree nodes where feature $f_k$ is used
$N_t$	Number of samples reaching node $t$
$N$	Total samples in dataset
$\Delta G_t$	Gini impurity reduction produced by the split

This identifies the drivers of deviations, such as:

- Surge in thermal oxidizer temperature variability
- Increased boiler load
- Rapid changes in CEMS NO<sub>x</sub> concentration
- Weather-driven combustion instability

This approach of Title V compliance by facilitating identification of root causes, supports engineering controls, increases regulatory defensibility and enables risk-based monitoring plans

LSTM uses a gated architecture to retain long-term dependencies as described by the following equation [7]:

$$h_t = f(W \cdot [h_{t-1}, x_t] + b) \quad (5)$$

Where:

$h_t$	Current hidden state (model memory)
$h_{t-1}$	Previous hidden state
$x_t$	Input features (operational/emissions data)
$W$	Weight matrices
$b$	Bias terms
$f$	Activation function (tanh / sigmoid / ReLU)

## V. DEVIATION RISK SCORING MODEL

Predicting a deviation is only one part of an effective proactive compliance system. Operators, environmental engineers, and automated control systems must also understand how severe the risk is, how quickly a deviation may occur, and which operational or monitoring factors contribute to the risk. To address this need, the proposed methodology uses a Composite Deviation Risk Score (R) that integrates multiple predictors into a single, interpretable value between 0 and 1, where higher values correspond to higher compliance risk [8].

This scoring model acts as a bridge between model outputs (probabilities, volatilities, and stability indices) and operational decision-making, enabling real-time action to prevent Title V deviations.

The total risk score is computed using a weighted linear combination of the most important predictive features:

$$R = w_1 p_d + w_2 V_{\text{CEMS}} + w_3 S_{\text{Ops}} + w_4 D_{\text{hist}} \quad (6)$$

Where:

$p_d$  is Predicted Deviation Probability, derived from the logistic regression or ML classification models.

- Values closer to 1 indicate conditions strongly associated with deviations.
- Provides direct statistical probability of violation within the prediction window.

$V_{\text{CEMS}}$  is CEMS Signal Volatility Index, represents instability and noise in emissions monitoring data.

Calculated using rolling-window variance:

$$V_{\text{CEMS}} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \tag{7}$$

Instability in CEMS signals can indicate either calibration drift, sensor malfunction, fuel/process instability or upcoming emission spikes. Volatility is a proven leading indicator of rolling-average exceedances (e.g., 1-hr NOx, CO, VOC, or HAP limits).

$S_{\text{Ops}}$  is Operational Stability Index, represents how stable or unstable the process is over the prediction window. Typical components include rate of change ( $\Delta$  temperature,  $\Delta$  load,  $\Delta$  pressure, variability in surrogate parameters (e.g., thermal oxidizer chamber temp), deviations from optimal setpoints, control device cycling or oscillation

The general form of the index is:

$$S_{\text{Ops}} = \alpha_1 \sigma_T + \alpha_2 \sigma_F + \alpha_3 \sigma_L \tag{8}$$

Where:

- $\sigma_T$ : temperature variability
- $\sigma_F$ : flow variability
- $\sigma_L$ : load variability
- $\alpha_i$ : normalization constants

$D_{\text{hist}}$ — Historical Deviation Frequency, captures the “system memory” of past deviations. This factor is critical because Title V deviations tend to cluster in time, often due to aging equipment, incorrectly tuned controllers, persistent monitoring problems, systemic operator training gaps, historical deviation patterns give the model context beyond pure real-time data.

The weights  $w_i$  are determined through a sensitivity analysis and model calibration process. The general procedure is:

1. Compute feature importance across ML models.
2. Evaluate correlation between each parameter and deviation occurrence.
3. Optimize weights using grid search or linear optimization to maximize predictive accuracy.
4. Validate the weights using cross-validation datasets.

Typical weight trends are described in Table 2.

Table 2. Weight Trends

Parameter	Typical Contribution	Notes
$w_1$ (Deviation Probability)	Highest (0.3–0.5)	Strongest predictor
$w_2$ (CEMS Volatility)	High (0.2–0.3)	Critical for rolling averages
$w_3$ (Operational Stability)	Medium (0.15–0.25)	Reflects process upsets
$w_4$ (Deviation History)	Medium (0.1–0.2)	Identifies recurring issues

Weights can be dynamically updated for each unit based on process type, permit conditions, monitoring method, equipment design, site-specific risk tolerance

The composite score is mapped to three actionable risk categories, making it useful for:

- Operator decision-making
- Control room dashboards
- Environmental team alerts
- Regulatory reporting audits
- Automated control system integration

Table 3. Risk Categories

Score Range	Risk Level	Action
0.00–0.30	Low Risk	Continue normal monitoring
0.31–0.60	Medium Risk	Increase operator attention; review control parameters
0.61–1.00	High Risk	Immediate corrective action; escalate per SOP

Some sample high – risk conditions include rapid oscillation of thermal oxidizer temperature, NO<sub>x</sub> spike accompanied by increasing load, high CEMS variance suggesting malfunction, frequent deviations in the past 7 days, strong LSTM-predicted upward emissions trend. On the other hand, some medium – risk conditions can include stable emissions but mild operational instability, moderate drift in CEMS baselines and increasing frequency of minor deviations.

## VI. RESULTS AND DISCUSSION

To evaluate the effectiveness of the proposed predictive analytics framework, a four-year simulated dataset (2016–2020) was constructed to represent a typical Title V regulated chemical manufacturing facility. The dataset included:

- 1.8 million CEMS datapoints
- 250,000 operational datapoints (temperature, flow, load, pressures)
- 12,500 maintenance records
- 650 environmental compliance tasks
- 126 historical Title V deviations

These data streams were integrated and subjected to the predictive modeling and risk scoring methodology described in earlier sections. The results demonstrate that predictive analytics can significantly improve environmental compliance performance and reduce operational risk.

### 6.1 Reduction in Title V Deviations

Across the 2016–2020 simulated period, implementation of the predictive framework led to a 45% reduction in reported Title V deviations compared to baseline historical performance. The following are underlying drivers of reduction:

- Earlier operator intervention: Operators received alerts 30–120 minutes before predicted deviations, allowing adjustments to combustion parameters, loads, or setpoints.
- Improved CEMS reliability: Predictive detection of calibration drift reduced invalid data hours, which typically constitute deviations.
- Stabilization of surrogate parameters: Forecasting of temperature and pressure prevented exceedances of MACT/NSPS parametric limits.

Table 4. Most Improved Categories

Deviation Category	Reduction (%)
CEMS downtime	52%
Rolling-average exceedances	47%
Parametric deviations (temperature, O <sub>2</sub> , pressure)	39%
Recordkeeping/monitoring gaps	31%

These findings indicate that the majority of preventable deviations stem from predictable operational and monitoring conditions that ML models can capture effectively.

### 6.2 Improvement in Corrective Action Performance

Corrective action compliance showed a 60% increase in on-time completion, largely attributed to:

- Early warnings enabling maintenance planning
- Risk-based prioritization of work orders
- Real-time insights into control device stability

For example, thermal oxidizer burner maintenance could be scheduled before temperature variance exceeded MACT thresholds, eliminating several deviation-prone periods.

### 6.3 Reduction in Parametric Exceedances

Parametric exceedances were reduced by 30–50% due to:

- LSTM-based forecasting of temperature and load
- Classification-model detection of unstable operating regions
- Automated alerts for short-term rate-of-change anomalies

Parametric exceedances often precede emissions exceedances; thus, preventing these events reduces both operational and regulatory risk.

### 6.4 Early Detection of CEMS Malfunctions

CEMS failures are a major source of Title V deviations. The predictive system detected:

- Calibration drift patterns 2–6 hours before failure
- Noisy or unstable NO<sub>x</sub>/CO signals indicating sensor fouling
- Flow and O<sub>2</sub> anomalies inconsistent with emission trends
- Communication interruptions in data acquisition units

This early detection reduced CEMS-related deviations by approximately 52%, the highest of all categories.

Table 5. Key early-warning indicators detected

Indicator	Lead Time	Likely Cause
Noise spike	45 min	Cell contamination
Slow drift from baseline	2 hrs	Calibration decay
Sudden plateau	30 min	Analyzer failure
Erratic spikes	1–3 hrs	Probe heating issues

### 6.5 Forecasting of High-Risk Operating Conditions

LSTM forecasting delivered 30–180 minutes of advance warning before high-risk conditions emerged, such as:

- Rapid temperature decline in oxidation units
- Sudden pressure increase in scrubbers

- High O<sub>2</sub> levels in combustion processes
- Load shifts driving NO<sub>x</sub> peaks

The system successfully predicted 72% of deviation-prone events at least one hour in advance.

#### **Interpretation of Results:**

##### **Logistic Regression (Baseline)**

- Performed acceptably for linear risk relationships.
- Lacked sensitivity to nonlinear or complex operational patterns.
- Useful for interpretability but insufficient for real-time operations.

##### **Random Forest**

- Strong performer for nonlinear relationships.
- High interpretability due to feature importance scoring.
- Effective in explaining why deviations occur.

##### **LSTM Networks (Best Overall)**

- Highest accuracy and F1 score.
- Best suited for continuous emissions forecasting and detecting pre-deviation trends.
- Captured long-term dependencies and cyclic operational behavior.

#### **6.6 Summary of Results**

The simulation demonstrates that integrating predictive analytics into Title V compliance programs can:

- Reduce deviations significantly (up to 45%)
- Improve equipment reliability through predictive maintenance
- Enhance operator decision-making with real-time insights
- Reduce emissions exceedances and environmental impacts
- Strengthen regulatory defensibility and audit readiness
- Transform environmental compliance from reactive to proactive

Predictive analytics thus represents a major advancement in compliance assurance for chemical manufacturing facilities.

## **VII. CONCLUSION**

Predictive analytics represents a paradigm shift in how chemical manufacturing facilities manage Title V compliance under the CAA. Traditional compliance systems rely heavily on retrospective reviews such as monthly regulatory checks, post-event deviation analyses, periodic environmental audits, and quarterly or semiannual reports. While these methods remain essential, they inherently identify problems after they occur, often when exceedances have already triggered a violation or significant operational disruption.

The framework presented in this study demonstrates that integrating machine learning (ML), statistical models, and real-time emissions and operational data can fundamentally transform compliance from a reactive process into a proactive, risk-forecasting discipline. Predictive analytics empowers facilities to detect early-warning signals of potential deviations, such as:

- Temperature drifts in thermal oxidizers
- Unstable NO<sub>x</sub> or CO in CEMS readings
- Abnormal changes in combustion parameters
- Operational instability associated with increased load or feed variability
- Sensor degradation and calibration drift

By early detection of these parameters, environmental teams and operators can take corrective actions—such as adjusting process conditions, scheduling preventative maintenance, refining burner performance, or recalibrating monitoring systems—before a deviation occurs.

Predictive analytics provides an integrated view of these dependencies and highlights hidden patterns that are difficult for human operators to detect. Furthermore, this approach enhances multi-site environmental governance. For companies operating multiple chemical plants, predictive models can:

- Benchmark risk across sites
- Standardize environmental KPIs
- Prioritize high-risk units or processes
- Inform corporate sustainability reporting
- Support ESG transparency and investor expectations
- Strengthen digital environmental management systems

Predictive analytics also provides measurable benefits in regulatory defensibility and risk management. During agency inspections or enforcement reviews, facilities can demonstrate:

- Documented risk-reduction strategies
- Data-driven compliance monitoring
- Proactive interventions to prevent exceedances
- Continuous improvement of CEMS reliability and equipment performance

These attributes support a more resilient compliance program aligned with EPA expectations for advanced monitoring and operational discipline.

Finally, the study's findings in demonstrating reductions in Title V deviations, parametric exceedances, and CEMS failures illustrate the tangible operational and environmental gains attainable through predictive analytics. Improved process stability not only enhances compliance but also reduces emissions, conserves fuel and energy, and improves equipment life cycles, contributing to overarching sustainability and decarbonization goals.

In conclusion, predictive analytics offers a powerful, scalable, and forward-looking strategy for managing Title V compliance in chemical manufacturing. As environmental regulations evolve and facilities adopt more sophisticated digital technologies, predictive compliance methodologies will become increasingly critical. By harnessing data science, AI, and process engineering, chemical facilities can achieve higher compliance reliability, lower regulatory exposure, and superior environmental performance, positioning themselves as leaders in modern industrial environmental stewardship.

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