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(REVIEW ARTICLE)

Integrating machine learning with environmental chemistry to forecast pollutant releases in coatings production

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Abstract

Coating and paint manufacturing is a large generator of toxic emissions and intricate waste streams, which consists of volatile organic compounds (VOCs), hazardous air pollutants (HAPs), heavy metals and strong wastes. These contaminants are highly dangerous to the health of the environment and human health and also cause issues with regulation under the regime of the Clean Air Act and the National Emission Standards for Hazardous Air Pollutants (NESHAP). The review studies models that can be used in predicting emissions, composition of waste streams, and process improvement by combining environmental chemistry with artificial intelligence (AI) and machine learning (ML) methods. Environmental chemistry has insight into the mechanistic understanding of the pollutant sources, transformation pathways and its analytical detection whereas AI can be used to enhance the predictive ability through multi-output modeling, deep learning architecture, and physics-informed frameworks. Examples of applications are VOC and particle emission modelling, heavy metals indoor wastewater residue forecasting, on-line estimation of process parameters to optimise the process to control emissions. This combination of AI and environmental chemistry has high promise in terms of proactive regulatory compliance, enhanced occupational health and sustainable manufacturing. Nevertheless, there are still issues of data quality, poor interpretability, scalability, and regulatory acceptability. The results highlight the change-making nature of AI-augmented environmental surveillance as a means of reducing the environmental impact of the coating and paint manufacturing industry.

Keywords: AI; Environmental Chemistry; Predictive Modeling; Coating and Paint Manufacturing; Volatile Organic Compounds; Hazardous Air Pollutants; Heavy Metals; Wastewater Treatment; ML; Sustainable Manufacturing

1. Introduction

Artificial Intelligence (AI) and Machine Learning (ML) have begun transforming various interdisciplinary fields by providing dependable solutions for data analysis, real-time decision-making, and autonomous navigation with an environmental solutions to the problems (Ademilua, 2021; Ufomba and Ndibe, 2023; Aemilia and Areghan, 2025a; Ndibe, 2024; Adjei, 2025b; Adjei, 2025a; Abolade, 2023; Ademilua and Areghan, 2022; Dada et al., 2024; Adjei, 2025c; Abolade, 2023; Ademilua and Areghan, 2025b; Utomi et al., 2024; Ndibe, 2025a; 2025b; Okolo et al., 2025; Umoren and Adukpo, 2025).

The paint and coating industry is one of the greatest consumers of pigments and organic solvents and hence significant generator of hazardous air pollutants (HAPs)- and volatile organic compounds (VOCs)- during formulation, application, and cleaning equipment. The common examples of HAPs are methylene chloride paint strippers and metal such as cadmium, chromium, lead, manganese and nickel that are released as aerosols in the spray atoms (U.S. Environmental

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Protection Agency [U.S. EPA], 2025; eCFR, 2025; Federal Register, 2021). In addition to air emissions, paint production and finishing activities produce complicated waste streams that include overspray particulates, gum- or solvents-contaminated rags, booth sludge and strong wastewaters. These waste waters can be described as highly containing chemical oxygen demand (COD), biological oxygen demand (BOD), suspended solids, colorants, surfactants, resins, and heavy metals due to pigments and additives (Nair et al., 2021; Aghbashlo et al., 2022). Such releases and wastes are highly regulated under Clean Air Act namely strategizing VOC and HAPs controls through national emission standards of hazardous air pollutants (NESHAP), New Source Performance Standards (NSPS) and Control Technique Guidelines (CTG) and co-complimentary industrial wastewater pretreatment standards, and predictive tools can be useful in complying and achieving eco-efficiency (U.S. EPA, 2025; eCFR, 2025).

The mechanistic basis of the source apportionment and fate of coating related contaminants is offered by environmental chemistry. Evaporation and emissions to the ambient air are controlled by solvent volatility and activity coefficients whereas aerosol physics dictates the distributions of droplets sizes and transport of metal bearing particulates of atomized coatings. Aqueous systems of pigment and resin behavior to partitioning and colloid chemistry is one of the primary factors in determining behavior, such as whether it is passively dispersed or gets lowered by treatment through flocculation and adsorption systems. Moreover, the process of reduction and oxidation and photolytic pathways lead to the degradation of binders, resin pieces, and additives (Dupont et al., 2020; Nair et al., 2021). The latest breakthroughs in chemometrics, including principal component analysis (PCA), partial least squares (PLS), and artificial neural networks (ANNs), have allowed scientists to disentangle these multidimensional and mutually reinforcing processes of the high-dimensional monitoring data, setting the basis of predictive modeling (Dupont et al., 2020).

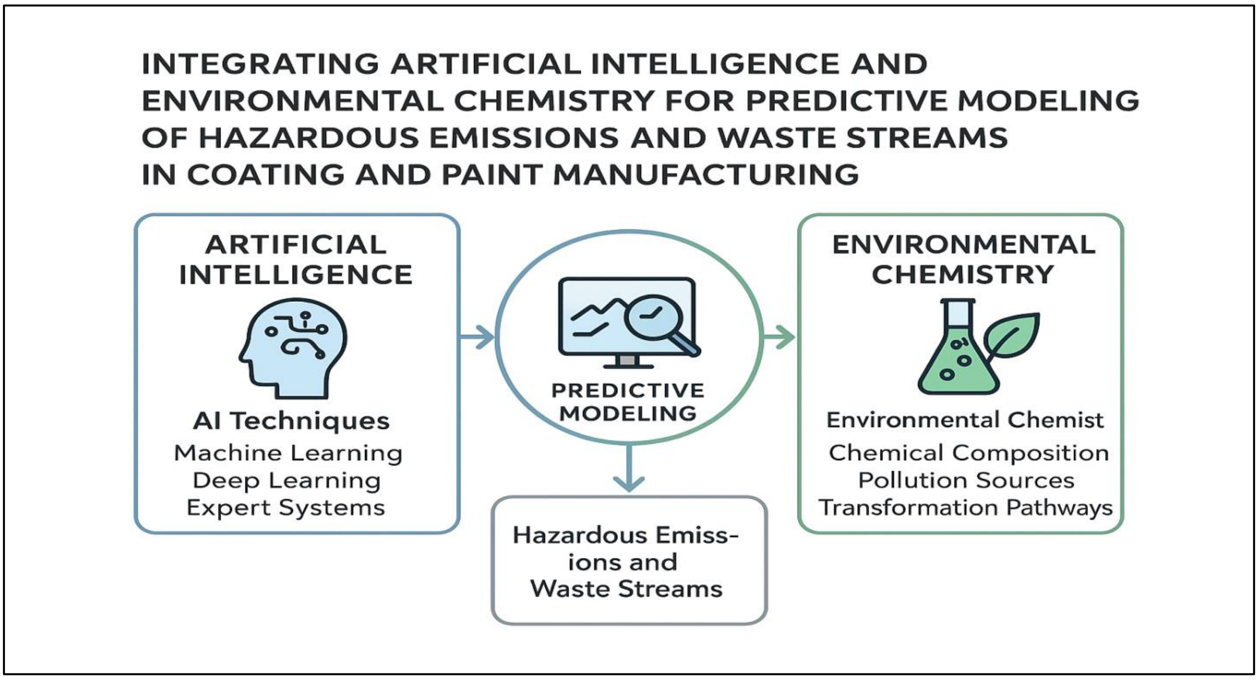

Figure 1 Artificial intelligence, predictive modeling and environmental Chemistry

Environmental monitoring in recent years, machine learning (ML) and artificial intelligence (AI) have demonstrated great promise in environmental monitoring, providing potent means of prediction of pollutants levels and discerning structure amidst noisy chemical data. The technologies allow proactive fortifications instead of post-factum reactions (Kavianpour et al., 2024; Rahman et al., 2024). In the case of air emissions, supervised learning models such as, random forest, support vector machines, gradient boosting, and deep learning architectures, have had high predictive accuracy responses where meteorological data, process surrogates, and/or real-time sensor measurements have been introduced. These plans might be adjusted to match that of coating booths and production plants (Rahman et al., 2024). In wastewater and solid waste streams, AI is used to improve spectrometric and chromatographic analytical methods (e.g., predicting retention times and collision cross sections in high-resolution mass spectrometry) and assists in dynamic, treatment-optimising soft sensing of COD and metals (Kavianpour et al., 2024; Dupont et al., 2020).

This review combines knowledge on environmental chemistry of emissions and waste streams of coating and paint manufacturing with innovative state-of-the-art AI and ML strategies to come up with predictive models. These objectives are to estimate the rate of VOC and HAP release rate in different formulation and operating environment, projecting the loads on the booth and wet-end wastes that can be optimally treated, and help to comply with regulatory requirements with minimum environmental impacts.

2. Environmental Chemistry of Hazardous Emissions and Waste Streams

2.1. Chemical Composition, Sources, and Transformation Pathways

A complex set of hazardous pollutants is generated in the paint and coating industry not only in terms of composition of the raw materials but also in the process itself. The kind of binders, solvents, pigment and additives are very important to the emissions. Specifically, organic solvent coatings contain especially high concentrations of volatile organic compounds (VOCs) and aromatics like benzene, toluene, xylenes (BTX), oxygenated compounds like alcohols, ketones and glycol ethers, and carbonyls such as formaldehyde and acetaldehyde (Atkinson and Arey, 2003; WHO, 2021). Polyurethane coatings is a special instance as they could release unreacted diisocyanates (e.g., toluene diisocyanate [TDI] and methylene diphenyl diisocyanate [MDI]) and amine catalysts which are very reactive and strong sensitizers of the respiratory system (NIOSH, 1996; OSHA, 2015).

The pigments and drying agents (driers), which are used to introduce trace metals, chromium, lead, nickel, and cadmium in paints, amongst others, are often toxic or carcinogenic. An example would be the anti-corrosive primers that contains hexavalent chromium that has been shown to emits Cr (VI)-containing particulate matter, the substance persists in the environment and is very hazardous in the workplace (IARC, 2012). The application procedures, like spraying, washing and cleaning, produce particulates, like overspray, and sanding and surface preparation produces fine dusts that consist of an inorganic, as well as organic, fraction. Such particulate matter usually has the potential of getting into the lowest parts of the lungs (PM2. ₵ and PM10) (NIOSH, 2003/2019). After their release, the transformation routes in the environment occur to a large number of these compounds. VOCs are oxidized in the atmosphere through contact reactions with hydroxyl radicals, ozone and nitrate radicals which results in secondary organic aerosols (SOA) and causes ground-level ozone pollution (Atkinson and Arey, 2003). Instead, metals can also be sequestered in soils and sediments where they can have long-term lasting effects as they bioaccumulate and eventually enter the food chain, posing chronic risks of exposure (WHO, 2021). Therefore, it is necessary to learn the main emissions of the plant and the process of their transformation in order to produce a correct assessment of risks.

Table 1 Summary of Major Pollutants, Their Sources, and Associated Impacts in the Coating and Paint Industry (Atkinson and Arey, 2003; WHO, 2021)

Pollutant	Primary Sources	Environmental Impacts	Health Impacts
Volatile Organic Compounds (VOCs)	Solvents in paints, thinners, drying processes	Formation of ozone and secondary organic aerosols	Respiratory irritation, carcinogenic risks
Heavy Metals (Pb, Cd, Cr)	Pigments, stabilizers, preservatives	Soil and water contamination, bioaccumulation	Neurotoxicity, kidney damage, developmental risks
Particulate Matter (PM)	Spray application, sanding, combustion	Air pollution, reduced visibility, climate forcing	Cardiovascular and pulmonary diseases
Formaldehyde and Benzene	Resin production, solvents	Photochemical smog, indoor air pollution	Carcinogenicity, eye and skin irritation
Wastewater contaminants	Equipment cleaning, production residues	Aquatic toxicity, eutrophication	Indirect health impacts via contaminated water

2.2. Analytical Methods for Detecting and Quantifying Contaminants

A large number of analysing techniques used in the characterization of hazardous emissions through paint and coating processes have been developed in the field of environmental chemistry. The compendium methods have been standardized in the U.S Environmental Protection Agency (EPA) specifically in gaseous pollutants like the VOCs. Method TO-15A codifies whole-air sampling in stainless-steel canisters and analysis by gas chromatography mass-spectrometry (GC/MS) (EPA, 1999b, 2019) and Method TO-17 codifies sorbent tube sampling, thermal desorption, and GC/MS analysis (EPA, 1999b, 2019). Regenerable carbonyl reactive compounds, such as formaldehyde and acetaldehyde, are usually determined using intakes on dinitrophenylhydrazine (DNPH)-cotted cartridges and the subsequent analysis extracted by high-performance liquid chromatography (HPLC/UV) as described in EPA Method TO-11A (EPA, 1999a).

Particulate matter: particulate matter is evaluated with the use of gravimetric techniques. In the case of stationary sources, EPA Method 5 protocols are given to collect isokinetic samples based on PM emissions in flue gases (EPA, n.d.-a). Typical occupational and ambient PM procedures implemented by NIOSH are the Method 0500 procedure to assess total particulates and the Method 0600 procedure to assess dust subfractions of this type, respirable (NIOSH, 2003/2019). The analysis of PM, especially metal fraction is undertaken by the acid digestion (e.g., SW-846 Method 3050B) followed by inductively coupled plasma - mass spectrometry (ICP-MS) or atomic emission spectroscopy (ICP-AES) according to EPA Methods 6020B and 6010C (EPA, 1996, 2014, 2024).

Under these methods, trace metals like Cr, Pb, Ni were detected at the low concentration level, which can serve as the foundation of mass balance as well as source apportionment. The novel developments in high resolution mass spectrometry and non-targeted analysis also increase the ability to identify previously unknown or emerging coating-related compounds whereas the chemometric tools, including the principal component analysis (PCA), can assist in the interpretation of multivariate information (Dupont et al., 2020). All these modes of analysis are essential in ensuring compliance, evaluating abatement technologies and finding devotion of top pollutants to be substituted or contained.

Table 2 Analytical Techniques for Pollutant Detection in Coating and Paint Industry (After Dupont et al., 2020; EPA, 1996, 2014, 2024)

Technique	**Target Pollutants**	**Strengths**	**Limitations**
GC-MS (Gas Chromatography-Mass Spectrometry)	VOCs	High sensitivity, excellent separation and identification of complex mixtures	Requires sample preparation; relatively high cost
ICP-MS (Inductively Coupled Plasma Mass Spectrometry)	Heavy metals	Multi-element detection, very low detection limits, high precision	Expensive equipment, requires skilled operators
XRF (X-Ray Fluorescence)	Metals in pigments and coatings	Non-destructive, rapid, minimal sample preparation	Less sensitive for trace levels; matrix effects possible
SEM-EDX (Scanning Electron Microscopy with Energy Dispersive X-ray)	Particulates (organic and inorganic)	Detailed morphology and elemental analysis	Time-consuming, requires vacuum conditions, not quantitative for trace gases
Gravimetric Analysis	Particulate matter	Simple, standardized, cost-effective	Provides only mass concentration, no chemical composition

2.3. Environmental and Health Impacts of Identified Contaminants

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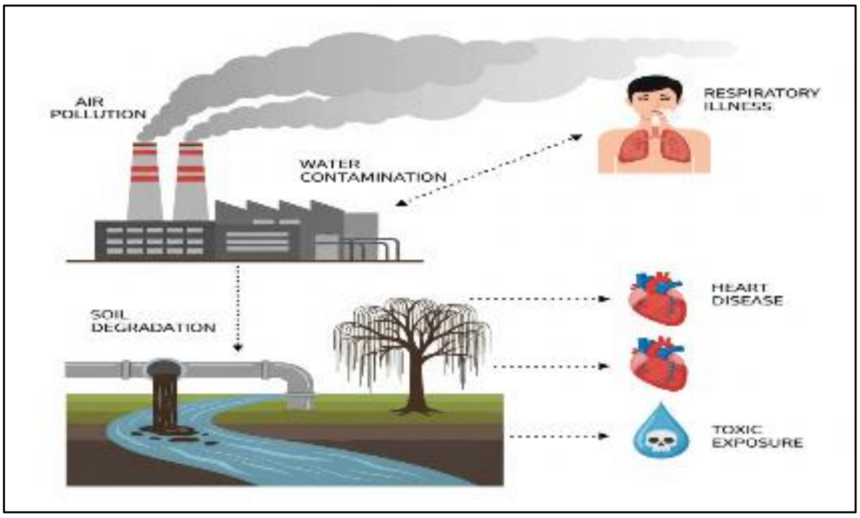

Figure 2 Environmental and health impact of contaminants

3. Artificial Intelligence Applications in Predictive Modeling

3.1. Overview of AI techniques for environmental prediction

The artificial intelligence (AIs) finding its way into the research of environmental chemistry is altering the way harmful emissions and waste streams are forecasted in the coating and paint industries. Machine learning (ML) Support vector machines, random forests, gradient boosting, and ensemble models have been used for modeling prediction of volatile organic compound (VOC) emissions, heavy metals and particulate matter (Agbehadji and Obagbuwa, 2024). Such models are good at processing massive, heterogeneous data such as chemical composition profiles or process parameters. More collectively, deep learning (DL), especially the recurrent neural networks (RNNs), long short-term memory (LSTM) architecture, and convolutional neural networks (CNNs), can have other benefits of capturing temporal and nonlinear changes between production variables and emission events (Chadalavada et al., 2025). However, contrastingly, expert systems, despite being rule-based, also fulfill an important purpose, which is the incorporation of domain knowledge regarding environmental chemistry, including reaction pathways of solvents, degradation products, or the regulatory limiting concentrations into predictive mechanisms (Eid et al., 2025). More and more, there also arise hybrid models integrating ML/DL techniques with expert systems, as they guarantee predictive accuracy among expert interpretability, which is essential, in particular, in regulatory compliance in chemical-intensive industries.

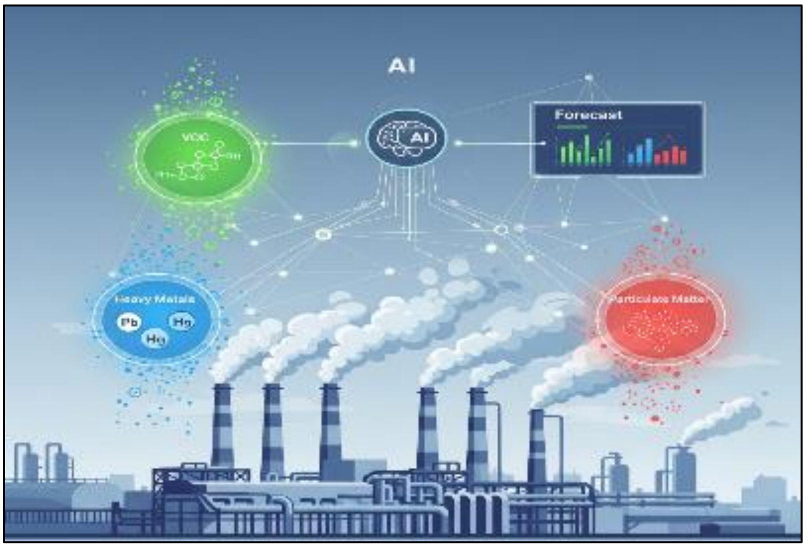

Figure 3 Integration of Artificial intelligence and environmental monitoring

3.2. Data sources and preprocessing

To ensure that AI models are efficient in predicting dangerous emissions, the models require multi-dimensional data that is of high quality. The process parameters which are critical in coating and paint production are the application pressure in the spray application, mixing ratios of resins and solvents, the ventilation rates and curing/drying temperature. There is a strong effect of these operational variables on the rate of release of VOC and the generation of particulate. Detailed information on pollutant composition is given by chemical profiles, which are based on laboratory characterization of the pollutants e.g., by gas chromatography= mass spectrometry (GC= MS) analysis to identify VOC speciation or inductively coupled plasma= mass spectrometry (ICP= MS) analysis to determine heavy-metal residues. Data on the pollutant's readings continuously (including stack gas, ambient air quality sensors, and constant particulate monitors) present dynamic information about changing pollutants under different production parameters (Rahman et al., 2024).

Preprocessing is a very important process when it comes to the integration of such datasets towards predictive modeling. The process of AI frameworks usually presupposes independent normalization of chemical concentrations, imputation of nonexistent sensor values, noise extraction, outliers' elimination, time-series data synchronization with particular production cycles (Chadalavada et al., 2025). During preprocessing, environmental chemistry knowledge can be used, including the recalculation of solvent reactivity indices, VOC ozone formation potential, or partition coefficients to augment theset to enhance the AI input features. Such combination of raw process data with chemically meaningful parameters makes the model easier to interpret and much more predictive.

3.3. Applications of AI in hazardous emission forecasting in coating and paint manufacturing

A number of AI solutions illustrate the possibilities of predictive models in terms of hazardous emissions in the coatings and paint industries. As an example, VOC mixtures have been predicted in the industrial process by multi-output machine learning models and have learned using co-emitted compounds and have decreased dependence on the continuous full-spectrum chemical analysis (Eid et al., 2025). All these applications underscore how combining AI and environmental chemistry benefits beyond amplifying the accuracy of predictive models, including compliance with regulation, waste management with a low environmental impact, and occupational health and safety. They include;

3.3.1. VOC Emission Forecasting paint application

VOCs are one of the most relevant hazardous pollutants which are emitted during coating and paint processes. The prediction of multiple concentrations of VOC species at the same time allows multi-output ML models in combination with co-emission patterns and solvent composition (Eid et al., 2025). Costly real time monitoring of the pollutants in the laboratory is minimised in such models because inferences about pollutant concentrations can be made using easy to access information about the processes. They can capture time-varying emission peak changes under different stages of paint curing and drying when used with the DL architectures such as LSTMs.

3.3.2. Predicting heavy metal residues in waste streams

Heavy metals commonly found in paint formulations include lead, chromium, and cadmium and finds its way to the wastewater or in sludge residue. Heavy metal loads can be predicted in the effluents using AI models trained on ICP-MS data, as well as taking into account operational variables: composition of pigments and waste treatment parameters. This aids the manufacturers to take constant control action in order to avoid crossing the thresholds and reduce the downstream environmental effects (Chadalavada et al., 2025).

3.3.3. Spray coating Particulate Matter (PM) Emission Monitoring

Fine particulates are produced due to spray application of coating which are hazardous occupationally and environmentally. Real-time sensor data have been used to present CNNs and hybrid ML models to forecast particle size distributions and concentrations. Through these models, more control of ventilation and protective equipment is made, and the exposure of the workers is minimized (Agbehadji and Obagbuwa, 2024).

3.3.4. Emission Control Emission-Real Time Process Optimization

In addition to projections, AI models would be used as a decision-supporting mechanism to reduce emissions. To take an example, hybrid ML-expert systems could prescribe ideal curing temperatures, volume of air circulation, or the use of solvents to reduce volatilizing organic compound emission and still guarantee quality of the product (Tang et al., 2022). Coating plants can achieve that by incorporating both predictive modeling and process optimization, which will help them shift to a more sustainable way of manufacturing.

3.3.5. Forecast Waste Water Monitoring

Most of the wastewater that is generated during the process of cleaning and rinsing in the manufacturing process of paint is composed of dissolved solvents, pigments and heavy metals. AI models can forecast effective chemical composition of effluents on the basis of production estimates and treatment station status to allow corrective action (e.g., pre-treatment of an effluent through appropriate pH adjustment, dosing with coagulants) prior to discharge (Rahman et al., 2024).

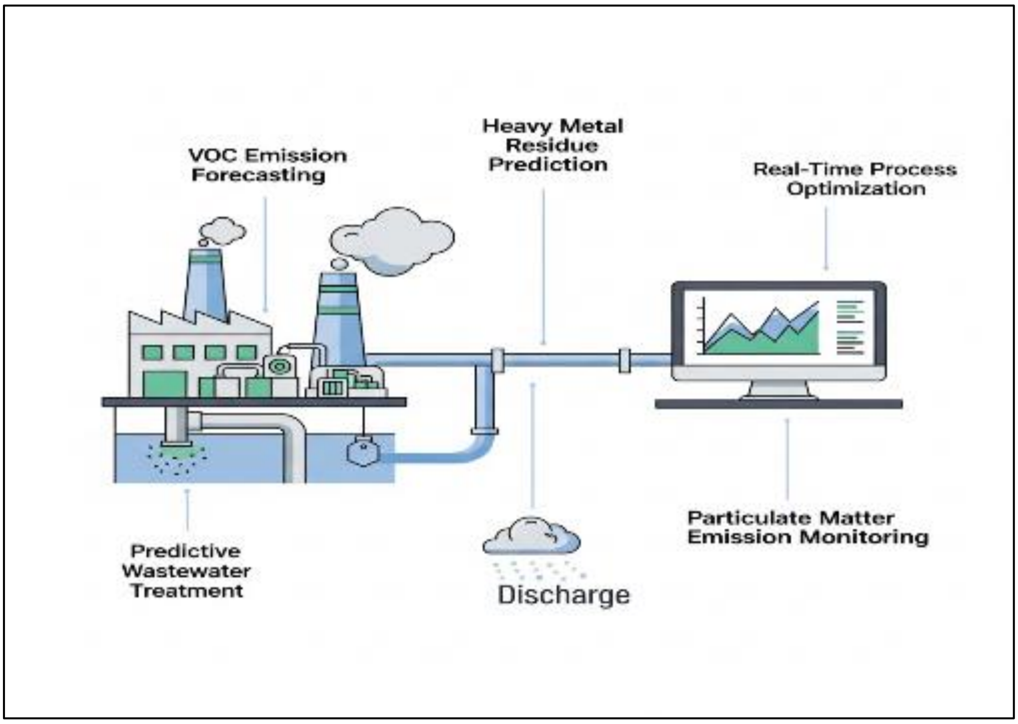

Figure 4 The different applications of AI in hazardous emission forecasting

4. Integration of AI and Environmental Chemistry

4.1. Frameworks for combining chemical analysis data with AI algorithms

Recent coating- and paint-industry emission modeling frameworks start by transforming the disparate outputs of the various analyses (GC-MS, GC-IMS, PTR-ToF-MS, sensor time series, process-control data) into harmonized sets of features via chemometric preprocessing (baseline correction, peak picking, alignment, deconvolution), and data fusion across instruments and stream-based processing (Houhou and Bocklitz, 2021). This preprocessing/ETL phase can in practical applications feed: (a) chemometrics + classical ML (PLS, random forest, gradient boosting) to generate interpretable regressions/classifiers; (b) deep-learning systems (CNNs using spectral or image like representations; RNNs/transformers using time-series process measurements) when a complex nonlinear pattern is desired; or (c) hybrid physics-informed deep learning models capable of learning a nonlinear pattern, into which the prior first-principles VOC emission model has been integrated with a lower-fidelity model Studies have revealed that two practical pipeline patterns are possible concerning paint and coating in particular:

(1) spectrum → chemometric features → ML model → pollutant concentration/source label, and (2) process parameters + limited measurements → multi-output ML (predict several VOCs simultaneously) → exposure/abatement alerts, enabling reduced reliance on full analytical panels in routine monitoring (Moura et al., 2024; Eid et al., 2025).

4.2. Model training, validation, and performance evaluation for accurate pollutant prediction

Training should respect the spatiotemporal and censoring reality of industrial VOC measurements: era or region to cross-validation training set, not naive random splits, to avoid autocorrelationâ€¦ On multi-output VOC tasks (as in coatings emissions where different co-emitted species vary together, so-called covariatory methods) multi-target regressors (e.g., multi-output Gaussian processes, CatBoost multi-target, multi-output neural nets) are able to exploit inter-compound correlations and can lead to better performance than fitting each pollutant separately (Eid et al., 2025). Highly effective deep models used in source-characterization (e.g. CNN+Class Activation Maps on PTR-ToF or mobile monitoring) are highly promising means of discovering diagnostic species or signatures, although, similar to most models, they will need careful external validation on difference production lines or factories, to demonstrate generalizability (Jing et al., 2024). Such recommended and recommended evaluation metrics include deterministic error (RMSE, MAE), explained variance (R?), and probabilistic/uncertainty measures (prediction-interval coverage, CRPS) in the case of uncertainties provided by the models, where the latter is essential in regulatory or occupational-safety contexts (Keith et al., 2021; Eid et al., 2025).

4.3. Benefits and challenges of interdisciplinary integration

4.3.1. Benefits

Integration accelerates detection of dangerous analytes (GC-IMS/GC-MS + ML), can enable surrogate monitoring (predicting difficult-to-measure VOCs based on more-easy proxies), autoprocess source apportionment based on high-resolution mobile or sensor networks, and can support real-time operational controls and abatement targeting in production lines-all of which minimize worker exposure and compliance risk (Moura et al., 2024; Eid et al., 2025).

4.3.2. Challenges

Data quality and representativeness: industrial coating data tends to be sporadic, instrument-specific, and biased on a formulation or production cadence basis; so pre-requiring massive data curation, calibration transfer, and domain adaptation. (2) Interpretability / regulatory trust: high-capacity models (deep nets, ensembles) pitch far better than simpler ones but risk being black boxes; explanationable AI (e.g. feature-importance, SHAP, CAM of CNNs) and physics-informed hybrids are needed to provide the right level of mechanistic insight and regulators acceptance. Uncertainty of scale and deployment: high frequency data on spectrum and processes require high-fidelity real-time pipelines, edge-computing to allow inference to run on-site, and maintenance/update strategies on data drifts as formulations or processes evolve. (4) Reproducibility and benchmarking: the field does not currently have widely agreed-upon benchmark datasets of coating-specific emissions, impeding cross-study comparison; we highly encourage open datasets, and commonly used methods of evaluation (Houhou and Bocklitz, 2021; Jing et al., 2024; Keith et al., 2021). The integration of domain chemists, analytical teams, ML engineers, and occupational health experts into the project lifecycle is hence necessary so as to transform model outputs to credible and subsequent policy and process decisions

5. Conclusion

The research points to the future of artificial intelligence (AI) and environmental chemistry being incorporated in the establishment of predictive environmental models of harmful substances or emissions as well as wastes associated with the coating and paint manufacturer industry. The synthesis of chemical characterization of volatile organic compounds (VOCs), hazardous air pollutants (HAPs), heavy metals, and particulates with machine learning (ML) and deep learning (DL) regimes can result in proactive emission prediction, optimized waste-minimization, and regulatory compliance refinement. Performance of AI-based predictive models has ranged from random forests and gradient boosting to physics-informed hybrid models and has shown considerable promise in predicting the rate of pollutant releases, tracking treatment performance, and prescriptively recommending how to operate the treatment facilities to achieve desired goals. Nonetheless, despite these developments, there are challenges still facing data quality, model interpretability, regulatory trust and scalability. To overcome these obstacles, they need to be solved by synergy between chemists, data scientists, process engineers, and regulators. All in all, the research shows that a predictive modeling approach driven by AI, with the input of environmental chemistry is a revolutionary way towards a sustainable manufacturing process and environmental footprints within the coatings and paint industry.

Recommendations

Using the findings of the research, some recommendations are formulated to key stakeholders. Industry practitioners must use AI driven monitoring and optimization tools to design efficient processes, compliance with regulations, lower the cost of operations as well as minimize environmental impact. Researchers must focus on the development of transparent and interpretable hybrid AI systems that could be validated on datasets of diverse multidimensional information. Good interdisciplinary cooperation among chemists, engineers, and data scientists will also be essential to make progress in predictive environmental modeling. Regulators are invited to facilitate open data sharing models and set standards regarding the acceptance of AI-based predictive systems in compliance monitoring and reporting. Policymakers ought to champion specific investments and funding models, promoting AI and environmental chemistry integration, especially in coursework that focuses on sustainable production and employee safety. Together, these suggestions can serve to hasten the movement to greener, data-driven, and more resilient practices in the coating and paint manufacturing industry.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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