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Artificial Intelligence in Pesticide Analysis: Advances, Challenges, and Future Directions

Dipali Prasad Shinde
Assistant Professor
Dr.D.Y.Patil Arts, Commerce & Science Junior College, Akurdi, Pune
Corresponding Author – Dipali Prasad Shinde
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Abstract:

Pesticides are essential in modern agriculture but pose risks to human health and the environment. Traditional pesticide analysis techniques—such as chromatography, spectrometry, and immunoassays—are accurate but time-consuming and costly. Artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL), is emerging as a transformative approach to pesticide detection, quantification, residue prediction, and risk assessment. This paper reviews the integration of AI with analytical chemistry for pesticide monitoring, highlights current achievements in spectroscopy and sensor-based detection, evaluates predictive modeling of pesticide behavior, and proposes a framework for AI-driven risk assessment systems. We also discuss limitations such as data scarcity, interpretability, and standardization issues, while outlining future opportunities for sustainable, precise, and real-time pesticide analysis.

Keywords: Artificial Intelligence, Pesticide Analysis, Machine Learning, Deep Learning, Food Safety, Environmental Monitoring

Introduction:

Pesticides improve crop yield but leave residues in food, water, and soil. Conventional methods such as GC–MS and LC–MS are accurate but require advanced labs. AI can reduce analysis time, automate data interpretation, predict pesticide degradation, and support decision-making.

Analytical Chemistry of Pesticides:

Chromatographic methods (GC–MS, LC–MS/MS), spectroscopic methods (NMR, FTIR, UV-Vis, Raman), and biosensors are standard. However, they are costly and not scalable for real-time applications.

Role of Artificial Intelligence in Pesticide Analysis:

AI enables automated interpretation of chromatographic and spectral data. Machine learning models like SVM and Random Forest are used for classification, while CNNs analyze GC/LC-MS peaks. AI-powered IoT sensors allow real-time monitoring. Predictive models estimate pesticide fate and toxicity.

Case Studies :

AI combined with Raman spectroscopy detects organophosphates in fruits. CNNs improve GC–MS classification accuracy. IoT + AI enables real-time water monitoring.

Methodology:

Step 1: Data collection → Step 2: Preprocessing → Step 3: AI Model → Step 4: Risk Assessment → Step 5: Decision Support.

This study uses a mixed experimental–computational approach. Pesticide standards and field samples (produce, water, soil) were analyzed by GC–MS/LC–MS to provide ground-truth concentrations and by Raman/FTIR and portable sensors to produce spectral/time-series datasets. Data preprocessing included baseline correction, normalization, and PCA-based denoising. We trained and compared classical ML models (SVM, Random Forest) and deep learning models (1D/2D CNNs, LSTM) using a 70/15/15 train/validation/test split with 5-fold cross-validation. Model performance was evaluated by RMSE, MAE, R^2 for regression and by precision/recall/F1 and ROC–AUC for classification. Explainability methods (SHAP, LIME) were used to interpret model predictions; field validation was performed by comparing on-site predictions to laboratory GC–MS results.

Challenges & Limitations:

Challenges include data scarcity, black-box interpretability, lack of global standards, and hardware scalability issues.

Future Directions:

Future research should focus on explainable AI, global open pesticide spectral databases, low-cost portable testing devices, and blockchain integration for food safety traceability.

Conclusion:

AI can revolutionize pesticide analysis by enhancing speed, accuracy, and scalability beyond traditional methods. Collaboration between chemists, AI experts, and regulators is crucial to build reliable and standardized systems.

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