Modeling charge particles dynamics and optimizing its collection efficiency by spherical collector using machine learning

Abstract

Particulate matter (PM) poses a serious threat to human health in both indoor and outdoor environments, necessitating the development of efficient, compact, and ozone-free air purification technologies. While electrostatic precipitators (ESPs) offer low pressure drop and high energy efficiency, conventional designs rely on corona discharge for particle charging, leading to ozone generation and reduced suitability for indoor applications. This thesis investigates a next-generation electrostatic collection strategy based on inductive charging and spherical collector geometry and develops a unified physics-informed and explainable data-driven framework to analyze, interpret, and optimize charged particle collection performance. The work begins with a detailed numerical and experimental investigation of charged particle dynamics in the non-uniform electric field generated around a spherical collector. High-fidelity simulations demonstrate that curved geometries produce strong spatial electric field gradients, resulting in coupled Coulombic and dielectrophoretic forces that significantly influence particle trajectories, energy dissipation, and deposition patterns. Particle capture is shown to be governed by a balance between electrostatic attraction, aerodynamic drag, viscous dissipation, and inertia, leading to size-dependent force-balanced capture regimes. Dielectrophoretic forces, although secondary in magnitude, are found to play a decisive role in enabling the capture of weakly charged or high-resistivity particles. A key limitation of spherical collectors, particle rebound due to oblique impacts, is then systematically analyzed. A three-dimensional numerical framework incorporating a sticking-rebound criterion is developed to quantify collision efficiency (ηc), rebound fraction (Rf), and overall collection efficiency (ηcol) under realistic flow conditions. Explainable machine learning (XAI) techniques, including SHapley Additive exPlanations (SHAP) and partial dependence analysis, are employed alongside a Light Gradient Boosting Machine (Light- GBM) surrogate model to reveal the relative influence of operating parameters and particle properties. The analysis establishes that rebound can account for 20–35% efficiency loss under unfavorable conditions and demonstrates that collision efficiency alone is insufficient to characterize collector performance. Distinct particle-size-dependent regimes are identified, with small and intermediate particles benefiting from strong electrostatic control, while larger particles exhibit inertia-dominated rebound behavior. Building on these insights, a surrogate-assisted multi-objective optimization framework is developed to simultaneously maximize collision efficiency and minimize particle rebound under polydisperse conditions. The trained surrogate model is used to explore an extended design space of approximately 5 × 105 data points, followed by clustering-based regime identification and evolutionary optimization. Pareto-optimal solutions are further ranked using a TOPSIS-based decision-making approach and locally interpreted using explainable machine learning tools to ensure physical consistency. The results demonstrate that optimal operating conditions are strongly dependent on particle size and that uniform operating strategies are inherently suboptimal for spherical electrostatic collectors. Overall, this thesis establishes a comprehensive and interpretable pathway from fundamental particle-scale physics to optimized system-level design for ozone-free spherical electrostatic collectors. By integrating high-fidelity simulations, explainable machine learning, and data-driven multi-objective optimization, the work advances both the mechanistic understanding and practical design of compact electrostatic air purification systems, providing actionable guidelines for next-generation indoor air quality control.