Seminar

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Institute for Plasma Research

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Title: Degradation of pesticide molecules by Cold Atmospheric Plasma: Reactive molecular dynamics insights

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Date: 16th May 2025 (Friday)

Time: 03.00 PM

Venue: Committee Room 1, IPR

Abstract

Water, soil, and food products often contain pesticide residues, which can accumulate in organisms and pose significant health risks, raising concerns about food safety. Cold Atmospheric Plasma (CAP) has shown promise in effectively degrading pesticides, offering high removal rates, energy efficiency, and environmental friendliness. In this study, we used Reactive Molecular Dynamics (RMD) simulations to explore the degradation mechanisms of the carbendazim pesticide molecule induced by reactive oxygen species (ROS). Our results reveal that ROS species such as OH, O, and O_3 trigger the breakdown of the toxic methoxycarbonyl group through hydrogen abstraction, dehydrogenation, oxidation, decarbonization, and decarboxylation reactions, leading to the formation of smaller molecules like CO_2. The destruction of this critical structure indicates a potential reduction in the biological activity of carbendazim.

Next, we turned our attention to organophosphorus (OPP) pesticides, which are the most widely used pesticides by farmers due to their effectiveness in controlling pests and their low cost. Using RMD simulations, we investigated the degradation of several organophosphorus pesticides specifically chlorpyrifos, diazinon, and quinalphos by reactive oxygen species (ROS). RMD simulations demonstrated the successful cleavage of the toxic phosphorothioate (P=S) bond, a key structural feature responsible for their activity as acetylcholinesterase inhibitors. We selected monocrotophos (MCP), an organophosphorus pesticide and insecticide, for further simulation and experimental studies, as it is commercially available in a formulation containing 53% MCP and 47% cyclohexane. MCP is commonly used to protect crops such as cotton, maize, paddy, sugarcane, groundnut, and various vegetables. Our RMD simulations revealed the degradation of the toxic dimethyl phosphate group $(O=P(OC)_2)$ and the vinyloxy substituent (C=C-O-P) through breaking of C-O bonds. We are currently planning to conduct experimental validation, including HPLC and GC-MS analysis, to confirm the degradation products predicted by our simulations.