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Predictive Modeling of Nanoencapsulated Pesticide Release for Optimized Agriculture and Reduced Environmental Impact

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Conventional pesticide application is highly inefficient, with less than 10% reaching target plants, with the rest leaving toxic residues that contaminate soil, groundwater and the food chain, harming non-target organisms. The use of encapsulated pesticides is a promising strategy to enhance agricultural yield while minimizing environmental impacts. One of the key advantages of nanoencapsulation is the controlled and sustained release of pesticides, in contrast to the direct release of conventionally-applied pesticides, which optimizes application efficacy and reduces unintended environmental exposure. Understanding the release kinetics of these nanoencapsulated formulations is crucial for designing efficient pesticide delivery systems. This study presents a comprehensive modeling approach to predict the release kinetics of pesticides encapsulated in porous hollow silica nanoparticles (PHSN). A major advantage of silica nanocapsules, in addition to their non-toxicity and biocompatibility, is their tunable morphology, allowing for structural modifications that can be tailored to achieve specific release profiles, thus enabling the development of nanocapsules suited to target pest requirements. The model integrates key physicochemical parameters of both pesticides and nanocapsules, such as the diffusion coefficient of pesticides, sorption interactions with the silica surface, shell porosity, shell thickness, and nanocapsule size. Model predictions are validated against existing experimental data on the release kinetics of various pesticides from porous silica nanocapsules. This modeling framework provides a mechanistic understanding of how various pesticides and nanocapsule material properties modulate pesticide release, enabling the rational design of nanocapsules to enhance pesticide efficacy. To demonstrate the efficacy of PHSNs in delivering azoxystrobin, a widely used fungicide, to plants, we compared PHSN-encapsulated and non-encapsulated azoxystrobin uptake in tomato plants via root and foliar application. Encapsulation significantly moderated the release rate, resulting in improved azoxystrobin tolerance in tomato plants treated by root application. Foliar application of nanoencapsulated azoxystrobin also led to controlled release and translocation compared to the non-encapsulated form, ensuring prolonged pesticide efficacy. The importance of rate of the pesticide release from PHSNs in controlling pesticide uptake and utilization efficiency underscores the importance of modeling in guiding the development of sustainable pesticide delivery nanocapsules that enhance crop protection while reducing pesticide losses.