

Insight into the adsorption properties of β -cyclodextrin/phillipsite organophilic composite for effective removal of toxic organophosphorous pesticides: kinetic and advanced equilibrium studies

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Table.S1. Nonlinear equations of kinetic, classic isotherm, and advanced isotherm models

Kinetic models		
Model	Equation	Parameters
Pseudo-first-order	$Q_t = Q_e (1 - e^{-k_1 t})$	Q_t (mg/g) is the adsorbed ions at time (t), and K_1 is the rate constant of the first-order adsorption (1/min)
Pseudo-second-order	$Q_t = \frac{Q_e^2 k_2 t}{1 + Q_e k_2 t}$	Q_e is the quantity of adsorbed ions after equilibration (mg/g), and K_2 is the model rate constant (g/mg min).
Classic Isotherm models		
Model	Equation	Parameters
Langmuir	$Q_e = \frac{Q_{max} b C_e}{(1 + b C_e)}$	C_e is the rest ions concentrations (mg/L), Q_{max} is the theoretical maximum adsorption capacity (mg/g), and b is the Langmuir constant (L/mg)
Freundlich	$Q_e = K_f C_e^{1/n}$	K_f (mg/g) is the constant of Freundlich model related to the adsorption capacity and n is the constant of Freundlich model related to the adsorption intensities
Dubinin–Radushkevich	$Q_e = Q_m e^{-\beta \varepsilon^2}$	β (mol ² /KJ ²) is the D-R constant, ε (KJ ² /mol ²) is the polanyil potential, and Q_m is the adsorption capacity (mg/g)
Advanced isotherm models		
Model	Equation	Parameters
Monolayer model with one energy site (Model 1)	$Q = n N_o = \frac{n N_M}{1 + (\frac{C1/2}{C})^n} = \frac{Q_o}{1 + (\frac{C1/2}{C})^n}$	Q is the adsorbed quantities in mg/g n is the number of adsorbed ion per site N_m is the density of the effective receptor sites (mg/g)
Monolayer model with two energy sites (Model 2)	$Q = \frac{n_1 N_{1M}}{1 + (\frac{C_1}{C})^{n_1}} + \frac{n_2 N_{2M}}{1 + (\frac{C_2}{C})^{n_2}}$	Q_o is the adsorption capacity at the saturation state in mg/g $C1/2$ is the concentration of the ions at half saturation stage in mg/L
Double layer model with one energy site (Model 3)	$Q = Q_o \frac{(\frac{C}{C1/2})^n + 2(\frac{C}{C1/2})^{2n}}{1 + (\frac{C}{C1/2})^n + (\frac{C}{C1/2})^{2n}}$	$C1$ and $C2$ are the concentrations of the ions at the half saturation stage for the first active sites and the second active sites, respectively
Double layer model with two energy sites (Model 3)	$Q = Q_o \frac{(\frac{C}{C1})^n + 2(\frac{C}{C2})^{2n}}{1 + (\frac{C}{C1})^n + (\frac{C}{C2})^{2n}}$	$n1$ and $n2$ are the adsorbed ions per site for the first active sites and the second active sites, respectively

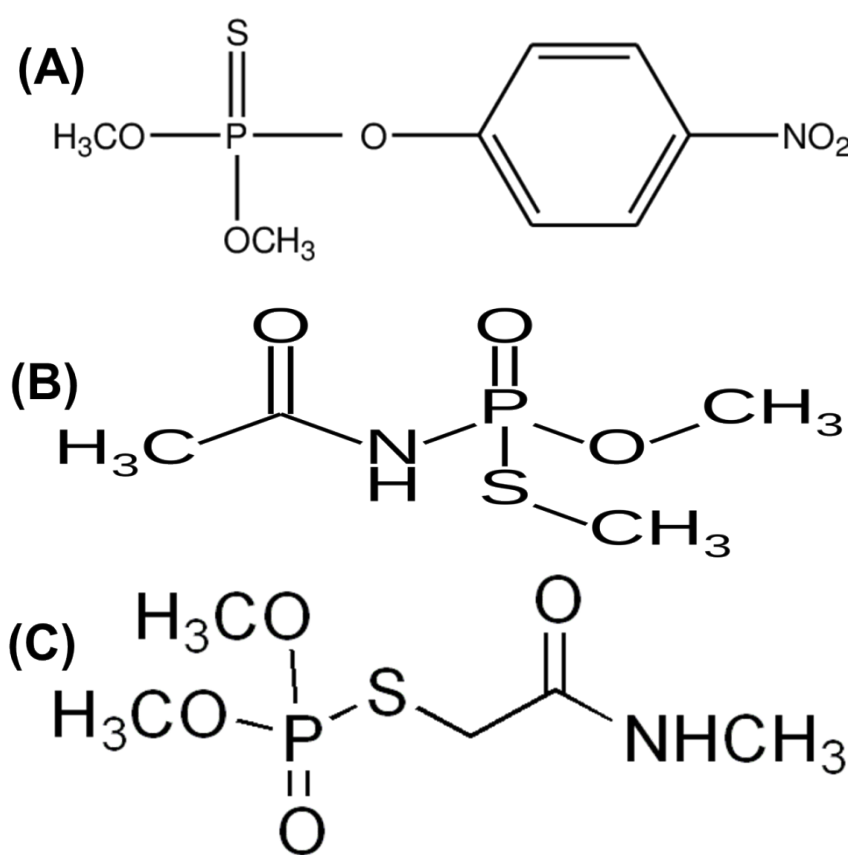


Fig.S1. The molecular structures of MPn (A), AC (B), and OM (C) pesticides

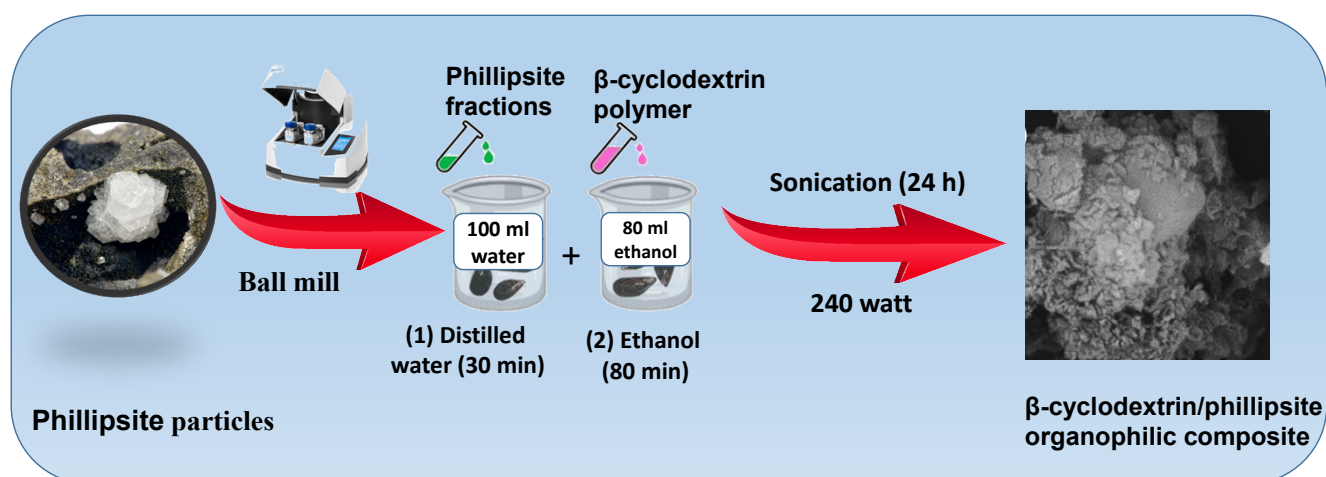


Fig.S2. Schematic diagram for the synthesis of CD/Ph composite

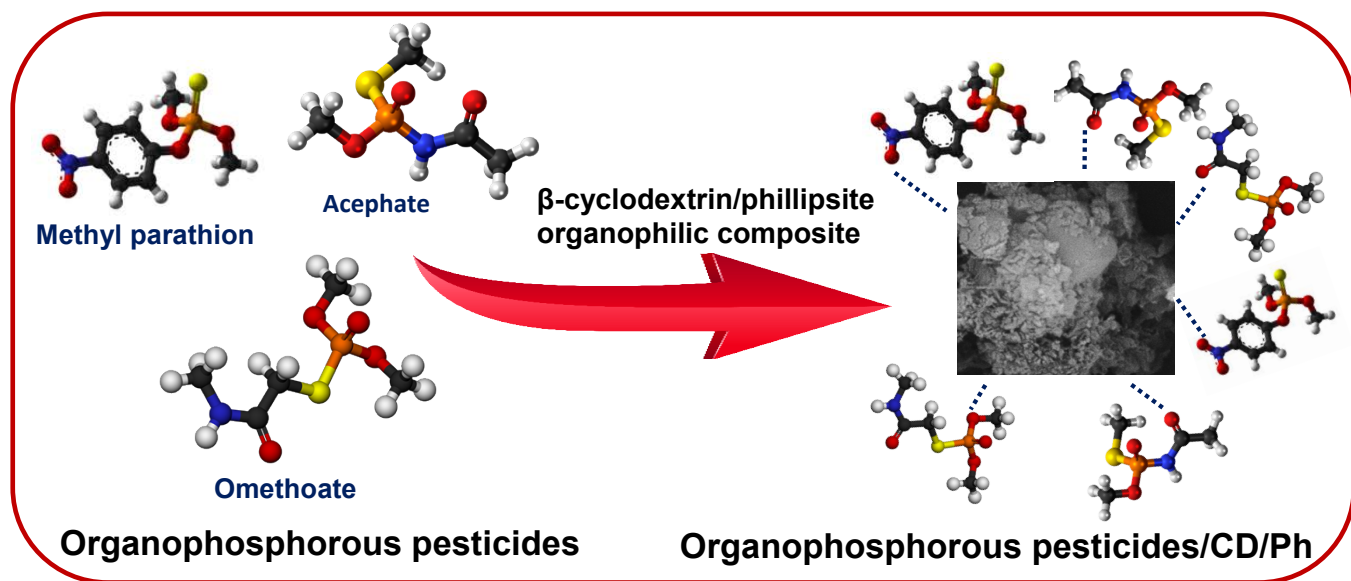


Fig.S3. Schematic diagram for adsorption of the different species of pesticides by CD/Ph composite