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Experimental and modelling study of CWPO over P-doped carbon black catalysts

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The catalytic wet peroxide oxidation (CWPO) of 4-nitrophenol (4-NP) with phosphorous doped carbon black catalysts (P-CB) was studied in the present work. The effect of reaction time (0-8 h), temperature (50-80 °C) and initial pH (2-4) on 4-NP removal and hydrogen peroxide consumption was investigated. Results exhibited the presence of an induction period showing an inverse dependence with the operating temperature and initial pH (pH₀). The power law model described well the reaction rates of 4-NP removal and hydrogen peroxide consumption. The slow initial rates were reproduced by taking into account the evolution of pH, expressed in terms of proton concentration in the model. Fitted kinetic equations and estimated parameter values are summarized in Table 1. As can be seen in Figure 1, the kinetic model properly describes the oxidation process.

Table 1. Kinetic model for CWPO of 4-NP upon P-doped carbon black

Kinetic equation	R ²
$-\frac{d[4-NP]}{[W] \cdot dt} = 237 \cdot \exp\left(\frac{-94 \text{ kJ mol}^{-1}}{R \cdot T}\right) \cdot [4-NP] \cdot [H_2O_2] \cdot [H^+]$	0.95
$-\frac{d[H_2O_2]}{[W] \cdot dt} = 65.6 \cdot \exp\left(\frac{-89 \text{ kJ mol}^{-1}}{R \cdot T}\right) \cdot [H_2O_2]^2 \cdot [H^+]$	0.88
$\frac{d[H^+]}{[W] \cdot dt} = 1.97 \cdot 10^6 \cdot [H^+]^{0.77}$	0.98

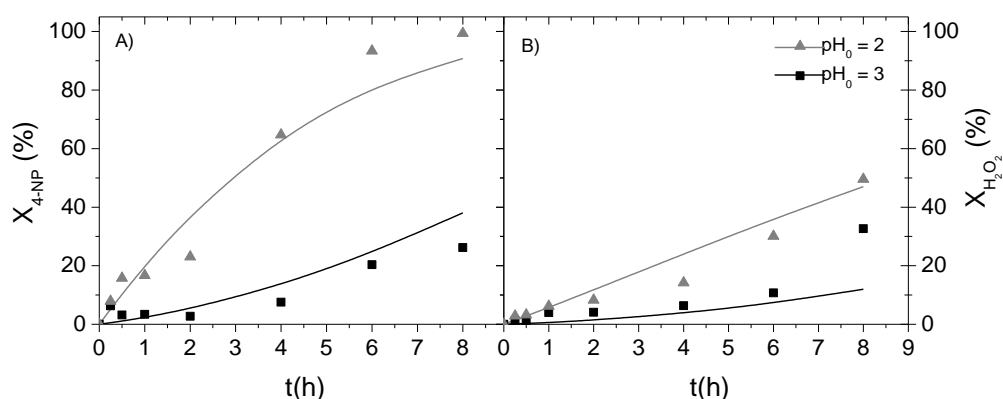


Fig. 1. Experimental data (symbols) and predicted values (curves) of 4-NP (A) and H₂O₂ (B) conversion in CWPO of 4-NP at 50 °C and 2.5 g_{cat} L⁻¹. C_{4-NP,0} = 5 g L⁻¹ and C_{H₂O_{2,0}} = 17.8 g L⁻¹

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