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KINETIC MODELLING OF WET PEROXIDE OXIDATION WITH N-DOPED CARBON NANOTUBES

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Carbon nanotubes (CNT) were tested as catalysts in the removal of 2-nitrophenol (2-NP) by catalytic wet peroxide oxidation (CWPO). The CNT materials were synthesized by catalytic chemical vapour deposition in a fluidized-bed reactor, as described elsewhere [1,2]. In order to synthesize a CNT with different characteristics, ethylene and acetylene were feeding as follows: 1) ethylene for 30 min (resulting in catalyst E30); 2) acetonitrile for 20 min, followed by ethylene for 20 min (A20E20); 3) acetonitrile for 20 min, followed by ethylene for 10 min (A20E10); 4) ethylene for 10 min, followed by acetonitrile for 20 min (E10A20); or 5) acetonitrile alone for 30 min (A30). These CNT were tested in CWPO adopting the experimental procedures reported in our previous studies [2-3] and at the following operating conditions: 50 ºC, pH_0 = 3.0, 0.25 g L^{-1} of catalyst, 0.5 g L^{-1} 2-NP and 1.78 g L^{-1} of added hydrogen peroxide (H_2O_2). Power-law kinetic equations were fitted to experimental data, following a similar statistical regression described elsewhere [4]. Results are depicted in Figure 1.

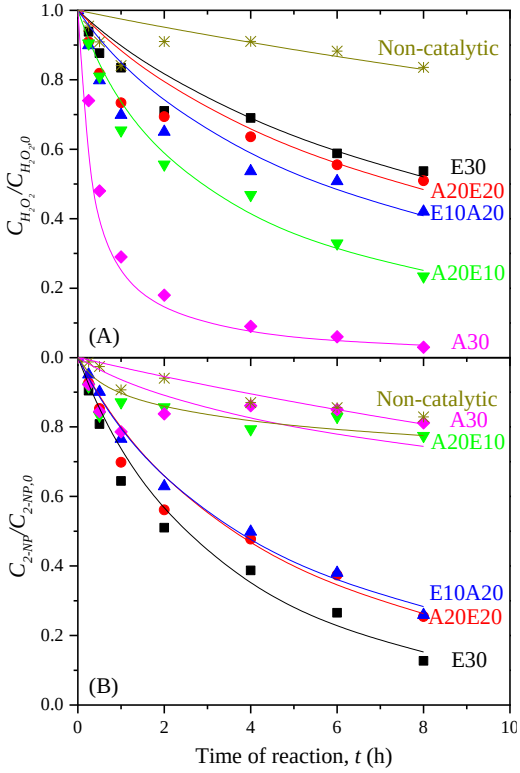

Figure 1. Experimental (symbols) and predicted (curves) evolution of (A) hydrogen peroxide and (B) 2-nitrophenol removals.

As can be observed, E30 was the most active catalyst for the degradation of 2-NP in CWPO. In addition, the H_2O_2 conversion obtained with this catalyst was the lowest, revealing a high efficiency in the H_2O_2 consumption (determined as converted 2-NP moles per consumed H_2O_2 moles). The power-law kinetic model predicts reasonably well the experimental data for all CNT samples. The equations of the model and the value of kinetic coefficients for each material are shown in Figure 2.

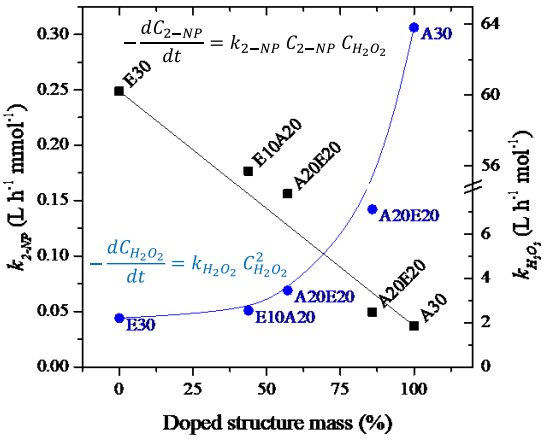

Figure 2. Kinetic constants as a function of the doped structure mass percentage in CNT catalysts.

As can be seen, coefficients were found to be related to the percentage of the doped structure in the CNT catalysts (determined by thermogravimetric analysis).

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