Ministry of Higher Education
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Experimental Study and Simulation of Advanced Oxidation Process for Phenol Removal in Wastewater

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ABSTRACT

Advanced oxidation processes (AOPs) are promised techniques for treatment of wastewater which containing refractory pollutants. In the present study, an experimental work and kinetic study with a simulation model were carried out to investigate the performance of a trickle bed reactor for phenol degradation in wastewater effluent from a petroleum refinery in Baghdad. Several process variables were investigated for their effect on the system performance. These selected variables are initial concentration of phenol (5 to 15 mg/L), temperature (120 to 160 ^{o}C), pressure (0.2 to 0.9 MPa), air flow rate (0.01 to 0.03 L/min), pH of solution(3 to 10), liquid flow rate ($0.6x10^{-3}$ to $1.66x10^{-3}$ L/min), and flow mode (co-current down-flow and up-flow). The experimental set-up was mainly composed of a stainless steel reactor of dimensions (13 mm ID x 160 mm long), packed with 5 gram activated carbon (0.8 mm particle diameter)as a catalyst. The optimum experiments were conducted using 3-level, 4-factor Box-Behnken design (BBD), with aid of modified of response surface methodology (RSM).

The result showed that the phenol degradation was enhanced by increasing temperature, pressure, and gas flow rate, while the initial concentration of phenol and liquid flow rate gave different images. High removal of phenol at about 97% was obtained at the optimum operating conditions ; LHSV=7 h^{-1}, temperature=160°C, oxygen partial pressure= 0.9 MPa, and phenol concentration= 5 mg/L. Down-flow mode proved to be more effective than up-flow mode for performance enhancement. Box-Benhken design (BBD) technique showed excellent results in choosing the best set of experiments with a quadratic second order polynomials response of phenol removal at a 99.63% correlation coefficient (R^2).

Kinetics of the process was found to behave as pseudo first order reaction with respect to phenol concentration, and 0.6 order with respect to oxygen solubility. Activation energy was equal to 77.7 kJ/mol, and pre-exponential factor was equal to($1.826*10^9$ L/kg-cat .h).When catalyst deactivation was taken into account, the oxygen order was equal to 1.4 and the frequency factor was about ($2.89*10^{10}$ L/kg_{cat}. h), also the activation energy was (97.677 kJ/mol).It was observed that the deactivation constant (k_{do}) was equal to ($2.9*10^{11}$ min^{-1}), and $E_{d_{ob}}$ was about (114.43 kJ/mol). The kinetic parameters (i.e., k and E) were estimated at each operating temperature using statistical analysis method. Catalyst effectiveness and deactivation rate were also estimated.

Simulation of the present AOP process requires a mathematical model that describes and predicts the process behavior. Dynamic modeling that predicts the concentration of phenol under study was formulated. The dynamic mass balance equations supplemented with the sub models of kinetic reaction were simulated by using MATLAB. To solve the non-linear complex system, a lumped model was utilized. Reasonable agreements were found when comparing the simulated results with the experimental data (mean absolute errors ranged between (0.002 to 0.005) for different operating conditions).

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