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Mineralization of Basic Blue 12 by heterogeneous Fenton like oxidation process: modelling, optimization, kinetic study and identification of intermediates.

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Abstract

In this work, artificial neural network and response surface methodology have been used to develop a predictive model for the simulation and optimization of total organic carbon removal of Basic Blue 12. The experimental data obtained from the total organic carbon removal of Basic Blue 12 was used to train an artificial neural network model with linear transfer function at output layer and a tangent sigmoid transfer function at hidden layer. Further, Box–Behnken design was employed to assess the individual and interactive effects of input process parameters on the total organic carbon removal of Basic Blue 12. First order kinetic model and lumped kinetic model was used to describe the reaction kinetics for the total organic carbon removal of Basic Blue 12. The high value of regression coefficient (R^2: 0.99) obtained for the lumped kinetic model suggested that the model was fitted well to the experimental data and the direct mineralization of Basic Blue 12 into CO_2 and H_2O could not be considered as the primary step. The intermediate compound formed during the total organic carbon removal of Basic Blue 12 were detected by liquid chromatography–mass spectrometry and were identified based upon the mass to charge ratio. The proposed mechanistic pathway based on identified intermediate compounds indicated that the degradation of Basic Blue 12 lead to formation of intermediates from destruction of conjugated structure of Basic Blue 12, and transformation of these intermediates into small molecules, which further mineralized to water and carbon dioxide.

Keywords: Basic Blue 12, artificial neural network, response surface methodology, lumped kinetic model, liquid chromatography–mass spectrometry