



UNIVERSITI  
TEKNOLOGI  
MARA

Institut  
Pengajian  
Siswazah

# THE DOCTORAL RESEARCH ABSTRACTS

Volume: 13, Issue 13

April 2018

# 13<sup>th</sup> ISSUE



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**Title :** PHOTOCATALYTIC DEGRADATION OF BENZENE-TOLUENE GASEOUS MIXTURE USING N, Fe-TiO<sub>2</sub> PHOTOCATALYST UNDER VISIBLE LIGHT: RESPONSE SURFACE METHODOLOGY (RSM) AND ARTIFICIAL NEURAL NETWORK (ANN) MODELLING

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Volatile organic compounds, VOCs such as benzene and toluene are hazardous to human health even when exposed at low concentration due to their carcinogenic impact. Recently, photocatalytic degradation has received great attention from researchers as one of the promising method to lower VOC concentration in the air. Common photocatalyst used for this process is titanium dioxide, TiO<sub>2</sub>. However, TiO<sub>2</sub> can only be activated under UV light range due to the wide band gap energy. Limited resources are the challenge faced in implementing photocatalytic degradation. This is because only 3% of the sunlight wavelength range is of UV light while the other 45% is of visible light. The conventional method, also known as the 'one-factor-at-a-time' is a common approach taken in photocatalytic degradation. This approach is usually difficult and the interaction between process parameters is complicated to interpret as it requires numerous experiments. Besides, the complexity of photocatalytic degradation also lies in predicting the removal efficiency of the pollutants. Hence, this study is attempted to modify the TiO<sub>2</sub> photocatalyst and to activate it under visible light wavelength range. The modified photocatalyst was applied in the photocatalytic degradation of individual benzene or toluene, as well as their gaseous mixture under irradiation of visible light. In this research, TiO<sub>2</sub> was modified by co-doping with nitrogen and iron elements, prepared using sol-gel method in order to activate the photocatalyst in visible light wavelength. The modified photocatalyst was characterized using XRD, BET surface area, UV-Vis DRS, and XPS. The synthesized N, Fe-TiO<sub>2</sub> was applied in the photocatalytic degradation, and tested with individual benzene or toluene, and benzene-toluene gaseous mixture under irradiation of visible light. To reduce the number of experiments, as well as to optimize the degradation process, response surface methodology (RSM) was applied for each photocatalytic degradation cases. Artificial neural network (ANN) models were also developed to predict the complexity of the photocatalytic

degradation process under visible light. It was found that N, Fe-TiO<sub>2</sub> photocatalyst is an anatase phase with crystal size of 19 nm and higher active surface sites. In addition, the energy band gap of N, Fe-TiO<sub>2</sub> photocatalyst is 2.33 eV, representing its ability to be activated under visible light wavelength region. RSM models have been developed to predict the removal efficiency of benzene, toluene and benzene-toluene gaseous mixture in order to optimize the responses. It was found that all independent variables that consisted of pollutant concentration, flow rate, and photocatalyst loading played a significant role in the degradation process which was evaluated based on the ANOVA, main effect, and variable interaction analysis. The optimum condition based on the RSM model of benzene-toluene gaseous mixture was 10 ppm (benzene concentration), 10 ppm (toluene concentration), 0.8 L/min (flow rate), and 25.54 (photocatalyst loading) which have successfully degraded 87.66% (desirable: 87.28%) and 90.83% (desirable: 89.95%) of benzene and toluene, respectively. Finally, the ANN models for individual benzene or toluene gas was 3-15-1, and benzene-toluene gaseous mixture was 4-15-2. The models were proven to have a good fit with high determinant coefficient, R<sup>2</sup> value for all cases, which is near to 1. The developed ANN models were good predictors for the application of the degradation process. The objectives of this research were successfully achieved, thereby marked the applicability of photocatalytic degradation of benzene-toluene gaseous mixture using N, Fe-TiO<sub>2</sub> photocatalyst under visible light irradiation. models (statistical and NARX model) predicted equally good performance ranging from 70% - 90% accuracy. Further analysis is required to test the developed model specifically for different river characteristics. However, the availability of data is a hindrance and to draw these findings, further recommendations are summarized for the validity of the derived equations.