

(第3号様式)(Form No. 3)

## 学位論文要旨 Dissertation Summary

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論文名:

(Dissertation Title) One-Step Phenol Production from Toluene and Benzene using In-Liquid Plasma

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This dissertation deals with two major process routes for the direct phenol production. The main objectives of the first route was to understand the process of converting toluene into phenol in a one-step process directly from a water-toluene mixture using the plasma in-liquid method. Experiments were conducted using 27.12 MHz radio frequency (RF) in-liquid plasma to decompose a solution of 30% toluene. Based on the experimental results as evaluated using the gas chromatography-mass spectrometry (GC-MS) along with additional analysis by the Gaussian calculation, density functional theory (DFT) hybrid exchange-correlational functional (B3LYP) and 6-311G basis, the phenol generated from toluene was quantified including any by-products. In the experiment, it was found that OH radicals from water molecules produced using RF in-liquid plasma play a significant role in the chemical reaction with toluene. The experimental results suggest that phenol can be directly produced from a water-toluene mixture. The maximum phenol yields were 0.0013% and 0.0038%, for irradiation times of 30 s and 60 s respectively, at 120 W.

The main objectives of the second route was to improve the yield of phenol from benzene-water mixed with single step process by using Dielectric-Barrier Discharge (DBD) plasma jet at atmospheric pressure. Maximum phenol yield and phenol selectivity this research were 28% and 82%, respectively. It was achieved when Ar/H<sub>2</sub>O flow rate 0 and flow rate benzene 10 μL/min at input power of 10 W. Moreover, in particular on the aspect of the conversion of benzene to produce phenol is better than the conventional process achievement cumene (5%). Maximum benzene conversion was 45% when ratio Ar/H<sub>2</sub>O flow rate in 10μL/min. This research has also shown the effects of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) with a focus on reactions involving the decomposition pure water (H<sub>2</sub>O). The amount of hydrogen peroxide increased when the flow rate ratio of Ar/H<sub>2</sub>O become small. When flow rate ratio of Ar/H<sub>2</sub>O is small or closer to 0 automatically the concentration of H<sub>2</sub>O in Ar/H<sub>2</sub>O that carrier pure water will be increased. OH radicals and hydrogen peroxide that are produced from water decomposition automatically increase if supply pure water or H<sub>2</sub>O concentration in gas Ar/H<sub>2</sub>O increase. With a high amount of hydrogen peroxide can be ascertained amount of supply of OH radical to react with the benzene molecule involved increases, and it is this, which is the key factor to get the high yield in phenol production.