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Studying competitive retention of phthalate esters by humic acid under multi-variable experimental design optimization: interaction between experimental factors

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ABSTRACT

Retention of phthalic acid esters (dimethyl phthalate (DMP), diethyl phthalate (DEP), dibutyl phthalate (DBP), diisobutyl phthalate (DIBP), and benzylbutyl phthalate (BBP)) by humic acid (HA) was addressed. The influence of experimental conditions: mass of HA, solution pH, temperature, and contact time on competitive uptake of esters were investigated and optimized under the frame of multi-variable experimental design. Conducting multi-factor process using appropriate design of experiment reduce the size of experimental work. Based on a proper experimental design, 11tests were required to investigate the uptake of phthalic esters from solution over the experimental conditions including HA mass (10, 25, and 50 mg/L), pH (6.0, 7.0, and 8.0), contact time (1.0, 5.0 and 16.0 h), and temperature (25.0°C, 35.0°C and 45.0°C). Mathematical relationships between independent variables (HA mass, pH, contact time, and temperature) and dependent variables (PAE uptake) were derived for each ester. For example, the DMP interaction by HA was presented as: DMP Retention (mg/kg) = 95.43 – 44.52 HA – 0.30 pH – 6.89 Time + 11.41 Temp + 0.97HA × Time – 1.31HA × Temp – 4.74 pH × Time – 5.05 Time × Temp. The above equation indicated a strong influence of single factors (HA mass, pH, contact time, and temperature) and the interaction terms (HA × Time, HA × Temp, pH × Time, and Time × Temp) on DMP uptake. Based on the outputs of the design, the average uptake of DMP was 95.43 mg/kg and better removal was achieved at lower HA dosages (10 mg/L) and higher temperature (45.0°C). Moreover, raising pH from 6.0 to 8.0 had a small influence on DMP uptake (the coefficient has a small and negative value –0.3). Although, contact time showed a negative influence on DMP removal (coefficient – 6.89), this factor has a positive influence but at longer contact time (HA × Time coefficient + 0.97). The negative influence of interaction terms (pH × Time and Time × Temp) expected the better DMP removal when these factors set at their opposite values. The adopted design of experiment has better performance to predict the influence of experimental factors compared with the classical signal-factor analysis.

Keywords: Design of experiments; Competitive interaction; Phthalate plasticizers; Humic acid

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