Abstract No: TC 10

Parameter Optimization and Kinetics Modeling for Biosorption of Methylene Blue Dye on *Artocarpus nobilis* Fruit Peel

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Dye removal through biosorption has not been extensively investigated at the industrial level, partly due to the lack of correlation between laboratory findings and requirements of large-scale applications. Bisorbents possess unique desirable characteristics for dye molecules to be attracted on to. In this respect, the present study aimed to evaluate the effectiveness and suitability of the powdered dried peel of *Artocarpus nobilis* fruit (710 μm < d < 1000 μm) for biosorption of methylene blue (MB) dye from synthetic solutions under static conditions through parameter optimization and kinetics studies. The optimum experimental parameters for over 90% removal of MB, determined through absorption measurements of equilibrated MB in solution phase (initial concentration = 10 ppm; solution volume = 50.0 mL) at its characteristic wavelength of 62.5 nm, are 0.150 g biosorbent dosage, 60 min shaking time, 15 min settling time and pH 4.5 – 9.3. Kinetics studies performed by varying biosorbent dosage (1.000 – 5.000 g), adsorbate concentration (2.5 – 13.0 mg L^{-1}) and solution temperature (27.0 – 51.0 ^{O}C), with other parameters being kept constant, demonstrate that the biosorption of MB follows pseudo-first-order kinetics with high regression coefficient values when compared to the pseudo-second-order model. Moreover, the pseudo-first-order rate constant determined for the above solution temperature range increased from 4.10×10^{-4} s^{-1} to 1.03×10^{-3} s^{-1} leading to an activation energy of 30.2 kJ mol^{-1} for the biosorption process. Further, the extent of adsorption of MB at equilibrium per unit adsorbent mass was found to increase with adsorbate concentration, decrease with biosorbent dosage, and remain almost constant with solution temperature in the above range. These are desirable characteristics for scaling–up of the proposed biosorption methodology for dynamic and proto-type studies for large-scale removal of MB.

Keywords: *Artocarpus nobilis*, biosorption, kinetics, methylene blue

Abstract No: TC 31

In silico study on thermal decomposition of polystyrene tetramer model compound

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The studies on the pyrolysis processes aid the development and use of pyrolysis technology for waste plastics. The present study investigated the thermal decomposition mechanism of the tetramer model compound of polystyrene by employing the density functional theory method at B3LYP/6-31G (d) level of theory. The calculated average bond dissociation energy of the backbone carbon-carbon bond, carbon-$carbon_{aromatic}$ bond, and carbon-hydrogen bond of the polystyrene model are 280.8 kJ/mol, 386.7 kJ/mol, and 664.4 kJ/mol, respectively. This suggests that the backbone carbon-carbon bonds are more likely to cleave in the thermal decomposition of polystyrene. Therefore, the initiation of the thermal pyrolysis mechanism of polystyrene occurs *via* carbon-carbon bond cleavage. Four possible pyrolysis pathways have