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Modeling the mass transfer kinetics of the grafting of 4-chloromethylstyrene onto polyethylene substrate

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There is a need for novel catalysts with better performance for biodiesel production. Some of the novel catalysts developed thus far are polymer based catalysts produced via graft polymerization processes. The production process of these novel catalysts have to be modeled in order to provide succinct data for use in designing systems for large scale production of these novel catalysts. The behaviors and performances of an ideal grafting of 4-chloromethylstyrene onto polyethylene substrates were predicted/discussed in this work using designed models. Conventional adsorption models developed and tested include Lagergren pseudo first-order model, Langmuir-Hinshelwood models, intra-particle diffusion model and Pseudo second-order diffusion model. Matrix Laboratory (MATLAB) was used as the model simulator due to its very broad and all-encompassing functions and capabilities. The models designed were compared and contrasted with one another and also with the experimental data for validation. Inferences were drawn on the basis of the findings and within the confines of the simplifying assumptions made. The validity of these models was tested on the basis of the R2 of linearized plots of the models. R2>0.9 was the criterion for validity. The Lagergren pseudo first-order model had the highest R2 values of 0.9034, 0.9400, 0.9798 and 0.9884 for the polyethylene samples at a reaction temperature of 60 °C. The Langmuir-Hinshelwood model was also satisfactory as it gave R2 values of 0.9282 at a temperature of 60 °C. The valid models were applied for process conditions other than those experimented upon and were found to give valid and reasonable results.

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