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Modelling of the Catalytic Hydrodeoxygenation of Bio-oil in Microreactors using Aspen Plus

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Microreactors have gained popularity in fuel production industries because of high surface area to volume ratios, enhanced mass and heat transfer, shorter residence times and a more sustainable practice. The catalytic hydrodeoxygenation (HDO) reaction of 4-Propylguaiacol (4PG) to 4-Propylphenol using pre-sulphided $NiMo/Al_2O_3$ catalyst has been investigated using a packed-bed plug flow microreactor using Aspen Plus. A steady-state, isothermal and pseudo-homogeneous microreactor was modelled using Peng-Robinson method and Langmuir Hinshelwood Hougen Watson kinetics. Operational factors such as reaction temperature, pressure, residence time, liquid flow rate and adiabatic conditions were investigated to determine their effects on conversion of 4PG. The results were then compared with experimental data from literature to assess the validity of the microreactor model. The model was aligned with experimental data for reactor conditions of 22.8 atm and 250-400 °C. Fig. 1 shows that the conversion of 4PG increases with temperature. The same trend was observed for pressure and residence time; however, 4PG conversion decreased with increasing liquid flow rate. Higher conversions can be achieved when adiabatic conditions are used as more heat is available for the reaction. The results obtained from the microreactor model show good agreement with experimental data. The differences in Fig. 1 are observed for temperatures >350 °C, because the results follow the % yield of other reaction products, which are not considered in the model, due to the lack of reaction kinetics available. To conclude, this model can be used to predict the hydrodeoxygenation of other components present in biomass-derived pyrolysis oils. Furthermore, there is a good possibility that microreactors can replace conventional macroscopic reactors to produce biofuels. They have the potential to enhance fuel output by means of scaling up, and they can be used for offshore fuel production.

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