Optimisation of Greener Alkene Epoxidation *via* Response Surface Methodology for Effective Separation of Epoxides from the Reaction Mixture

Md Masud R. Bhuiyan[1], Basudeb Saha[1]
[1]*School of Engineering, Lancaster University, Lancaster LA1 4YW, UK*

Abstract

Alkene epoxidation has been established as an important process for chemical synthesis as the resultant epoxide acts as a raw material or intermediate that can be transformed into many useful substances such as plasticizers, perfumes, and epoxy resins. The conventional epoxidation process involves stoichiometric peracids as oxidising agents, but it is not environmentally friendly. In contrast, polymer-supported heterogeneous catalysts with *tert*-butyl hydroperoxide (TBHP) as an oxidant have demonstrated strong catalytic activity and product selectivity. In this study, an efficient and selective polybenzimidazole-supported molybdenum (VI) complex (PBI.Mo) was used for the batch epoxidation of 1,5-hexadiene and 1,7-octadiene. Response surface methodology (RSM) using Box-Behnken Design (BBD) was employed for designing experimental runs and studying the interaction effect of different variables including reaction feed molar ratio of alkene to TBHP, reaction temperature, catalyst loading, and reaction time on the percentage yield of the reaction. Batch epoxidation of 1,5-hexadiene and 1,7-octadiene with TBHP as an oxidant in the presence of polymer-supported Mo(VI) catalyst was conducted in a classical batch reactor. The products were separated from the batch reaction mixtures and collected at regular intervals from reaction mixtures and analysed using Shimadzu GC-2014 gas chromatography. Design Expert software was used to develop the numerical optimisation step by combining the desirability of each independent variable into a single value and then searching for optimum values for the response goals. To validate the optimal response values of the predicted quadratic equation, batch experiments were performed at optimum conditions. The reusability studies of PBI.Mo catalysts have been performed in order to reduce production costs and consider large-scale industrial applications. Experimental results for epoxidation reaction showed that the catalyst could be used several times without any appreciable decrease in the conversion of TBHP for batch experiments. This study demonstrates that PBI.Mo complex could be used as an effective catalyst for a greener and more efficient epoxidation of alkenes with TBHP as an oxidising reagent.

Keywords: *tert*-butyl hydroperoxide (TBHP), epoxidation, batch reactor, polymer-supported Mo(VI) catalyst, Response surface methodology (RSM), 1,5-hexadiene, and 1,7-octadiene.