Modeling the Synthesis and Application of Polymeric Catalysts

Leandro G. Aguiar, William M. Godoy, University of São Paulo, Lorena / Brazil.
Nuno A. B. S. Graça, Alírio E. Rodrigues, University of Porto, Porto / Portugal

ABSTRACT

Two modeling approaches were developed in order to quantitatively assess the effect of crosslink density on the catalytic activity of sulfonated styrene-DVB resins: (I) a model considering a fraction of inaccessible catalytic sites in the resin, and (II) a model that describes a variable reactivity along the resin in function of the chain sequences distribution. A styrene-divinylbenzene copolymerization model was developed in Scilab®, taking into account a balance of sequences between crosslinks (SBC). The SBC length distribution characterizes the degree of crosslinking of each resin, and this information was used in models I and II for the simulation of catalyzed reactions. A second order pseudo-homogeneous rate equation was considered in both models, representing esterification reactions catalyzed by the acidic resins. The Model I revealed that the fraction of inaccessible sites ranged from 10% to 72% of the total sites for resins with 4% and 20% DVB, respectively. This simplified approach provided that the sites contained in SBCs with 6 or less monomer units are inaccessible for the catalyzed reactions studied herein. A linear correlation for the fraction of inaccessible sites as function of sequences distribution was proposed and validated, providing $R^2 = 0.992$. The Model II presented a limit of 50 repeating units between cross-linking points, from which no reactivity variation is expected to occur. For SBCs with less than 50 monomer units, the reactivity varied exponentially as a function of SBC length. The rate constants obtained in this modeling study are coherent in comparison with literature data, and the other parameters were consistent for the same type of resin. The models were validated with experimental data from different authors and provided fair agreements.

Keywords: polymeric catalyst, resin, esterification, accessibility.

Reference

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