Sulfonation of Poly (styrene-co-ethylene glycol dimetacrylate): Experiments and Mathematical Modeling

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Abstract

Sulfonated Styrene-co-Divinylbenzene (Sty-co-DVB) particles have been widely used as catalysts in various processes. Other crosslinking agents, poorly studied in the literature, have similar properties and can also be used for the same objective. This study aims to produce sulfonated polystyrene particles crosslinked with Ethylene Glycol Dimethacrylate (EGDMA) and to develop a mathematical model of the sulfonation process. Sty-co-EGDMA particles produced with different combinations of monomer fraction, percentage of crosslinker and inert solvent fraction were sulfonated with concentrated sulfuric acid in a heated reactor with temperatures in the range 50 - 80 °C. The mathematical modeling of the process was carried out based on the shrinking core model derived from the continuity equations for spherical coordinates. Ion exchange capacities, kinetic constants and diffusion coefficients were determined. The experimental results showed higher ion exchange capacity (3,40 meg/g - 4.00 meg/g) at lower temperatures and higher crosslinker contents. This behavior is the opposite observed for Sty-co-DVB particles found in literature and may be explained by the EGDMA chain size that is greater in comparison to DVB, allowing higher accessibility to the active sites. The diffusion coefficients were higher when higher crosslinker amounts were used. Again, the chain extent may be influencing on mass transfer coefficients along the particles. However, for greater temperatures and smaller crosslinker content, the particles showed a higher degradation. Samples collected with more than 90 min of sulfonation reaction showed reduced ion exchange capacity and higher degradations.