Modeling of hydrogen peroxide-based epichlorohydrin process

김우현, 윤좌문, 김 영[1], 박정호, 박선원*, 정기택[2], 우경섭[2],
이용화[2], 김세헌[2]
KAIST; [1]한국기계연구원; [2]한화석유화학(주)
(sunwon@kaist.ac.kr*)

A liquid-phase epoxidation process using hydrogen peroxide (HP) and titanium silicate (TS-1) is an eco-friendly technology to produce epichlorohydrin. In this work, a mathematical model is built to predict catalyst deactivation, temperature profile, as well as time-varying conversion and selectivity of a packed-bed tubular reactor using HP and TS-1. The reaction mechanism of this process is selected as the Eley-Rideal mechanism and the pertinent kinetic parameters are estimated by genetic algorithms. The optimal operating temperature is identified to maximize catalyst activity in a long-term operation by controlling hot spots of the reactor. In addition, the optimal length of the reactor is also determined to maintain desired conversion and selectivity. Simulation results present both conversion and selectivity could be maintained above 96% during 2,000 hours for the optimally-sized reactor operating at identified optimal conditions.

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