Multiscale simulation of homopolypropylene process on CAPE-OPEN platform

kofi oware sarfo, 이재철[1], 김신혁, 오 민*
한밭대학교; [1]이벤시스코리아
(minoh@hanbat.ac.kr*)

The progressive demand from the market for particular properties has compelled the improvement of the polypropylene manufacturing process. This project resolves this by predicting the behavior of the process using mathematical models and simulations. Hence, simulations were done at the microscale level having the reaction kinetics, the macroscale level involving the reactor and multiscale level adding various units in the flowsheet, simultaneously via an interface. A dynamic model was made and simulated expressing liquid-phase propylene homopolymerization in a stirred reactor with Ziegler-Natta catalyst on the gPROMS software. Moreover, the method of moments was employed to predict the molecular weight, polydispersity and melt indices. The steady state model was connected by CAPE-OPEN interface to PRO/II modeling software. Meanwhile, models of accessory equipment for the homopolypropylene process were connected in the PRO/II software and simulated with a reference data for the validation of the model. Simulation results were consistent with reference data with a reasonable percentage error.