

Modeling of Copolymerization of Carbon Dioxide and Epoxide for Producing Polycarbonates

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Carbon Capture and Utilization(CCU) technology has become significant against the deterioration of global warming. Production of polycarbonate through the copolymerization of carbon dioxide and epoxide is one of the promising routes in the CCU field. It is eco-friendly in that polycarbonate product has biodegradable property while using carbon dioxide as feedstock. Notably, the modeling of polymerization reactor has a complexity due to its large scale of equations involving the system which depend on the time variable. Since polymerization reaction is necessary to describe with dynamic modeling based on reaction kinetics, Method of Moments(MoM) is used to simplify a theoretically infinite number of mass balance equations for polymer chains into a smaller set of equations. The modeling under (salen)CrX catalyst is simulated by Python, and sensitivity analysis is undertaken based on different operating conditions(e.g. reactor temperature, feed rate).