

Public Abstract

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Title:MODELING AND EXPERIMENTAL STUDY OF POLYURETHANE FOAMING REACTIONS

Polyurethanes are very important polymers and are used in a wide range of applications. A theoretical model was developed to simulate polyurethane foaming reactions. In the model, multiple ordinary differential equations were solved by MATLAB program and the model was able to predict temperature, foam height and concentration profiles. This model can provide a better understanding of fundamental polyurethane chemistry and the foaming process.

Further modeling and experimental studies were performed to improve accuracy and to expand capability of the simulation program. Impact of side reactions, impact of catalyst and surfactant concentrations and impact of catalysis poisoning were taken into consideration and included in the model. The revised model was able to predict bubble radius, inside bubble pressure, vapor pressure of pure isocyanate as well as more reasonable temperatures, foam height, and concentration profiles. Reaction kinetics and thermodynamics parameters used in the simulation program were verified by experimental and/or computational methods respectively.

The use of simulation offers a way to control the complexity and transform materials design, just as process simulators have transformed engineering design. This perspective presents a case that simulation is ready to change the way we research, develop, and design polyurethane formulations.