Public Abstract
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Graduation Term:SP 2013
Department:Chemical Engineering
Degree:MS
Title:POLYURETHANE RIGID FOAMS MODELING PROJECT

Polyurethanes are very important polymers and have a surprising array of commercial applications. The polyurethane polymer-forming reaction occurs between an isocyanate and an alcohol. To make foams, the polyurethane polymer must be expanded or blown by the introduction of bubbles and a gas. A convenient source of gas was the carbon dioxide produced from the reaction of an isocyanate group with water.

A theoretical model was developed to simulate the polyurethane foaming process for a rigid foam. In the model, multiple ordinary differential equations were solved by MATLAB and the model was able to predict temperature profiles by inputting foam recipe information. This initial study on foam modeling focusses on reaction kinetic parameters that were fitted to experimental temperature data as a function of time. The modeling was able to accurately model temperature profiles of single-polyol polyurethane formulations and was able to accurately predict temperature profiles of mixtures based on pure component kinetic parameters. A primary goal of this work is to expedite the ability to develop new foam formulations by simulation - especially for incorporation of new bio-based polyols into formulations. In additional, there was a research program to predict the density of the foaming studies in the lab and then the results are to be used to revise the formulation to obtain a density identical to the base case.

The MATLAB model based on the simultaneous solution of several differential equations was developed further to include the impact of catalyst loading for the reactions and physical processes of a urethane box foaming process. Experiments with different amounts of catalyst loading were conducted to fit the model parameters for this thermoset polymerization. The revised model improves the versatility of simulation for predicting temperature profiles, viscosity profiles, and densities during urethane foam-forming processes.

In addition, becoming knowledge on likely fates of unreacted isocyanate and developing experimental plan to evaluate reactions with excess isocyanate in solvents are significant. ASTM isocyanate titration was applied to measure isocyanate content in system during foaming process. Experiments with different amount of catalyst were carried out to verify accuracy of the model. Kinetics parameters relate to side reactions will be obtained by fitting modeling results to experimental data.