

POLYURETHANE RIGID FOAMS MODELING PROJECT

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ABSTRACT

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.

The MATLAB model was developed further to include the impact of catalyst loading for the reactions. 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.