SIMULATION AIDED ANALYSIS AND EXPERIMENTAL STUDY OF POLYURETHANE POLYMERIZATION REACTION AND FOAMING PROCESS

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ABSTRACT

A MatLab simulation model was developed to simulate polymerization reactions, gel point times and foam formation. The simulation is based on the simultaneous solution of typically 25-80 ordinary differential equations that describe elementary reactions, energy balances, and mass transfer. Laboratory polymerization experiments were performed to evaluate the accuracy of the simulations, including setting up experimental systems and measurement of temperature, height, and viscosity profiles of the urethane systems.

The performance of physical and chemical blowing agents were simulated with mass transfer of the blowing agent estimated as a function of reaction temperature and resin viscosity. The simulation code of polyurethane reactions allows the studying of variables that are impossible to obtain in labs like the rate of foam's cell growth and pressure inside the cells. Also, simulation provides insight into mechanisms such as how attaining a reasonable maximum reaction temperature is important to properly cure foams and avoid foam shrinkage.

The impact of mass transfer limitation of the reacting moieties was successfully simulated based on three fundamental approaches. Further modeling shows the ability to reduce the number of parameters used for simulating urethane reactions by considering the viscosity dependent term for the frequency factor of Arrhenius equation.

Finally, the simulation studies of this research provide fundamental insights into the mechanism of homogeneous and catalytic reactions. This research process places high demands on identifying and testing highly-impactful fundamental mechanisms during polymerization that have not previously been identified.