Public Abstract
First Name:Huaqi
Middle Name:
Last Name:Wang
Adviser's First Name:Galen
Adviser's Last Name:Suppes
Co-Adviser's First Name:
Co-Adviser's Last Name:
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Title:A STUDY OF POLYURETHANE POLYMERIZATION
VIA MODELING AND EXPERIMENT

This thesis is on the topic of modeling thermoset polymerization. More specifically, Chapter 2 is a detailed study of isocyanate concentration profiles with the goal of validating modeling work that was based on temperature profiles for polyurethane thermoset polymerization. Chapter 3 is on an extension of the modeling methods to resin polymerization of unsaturated vegetable oils.
On the work related to polyurethane thermoset polymerization, a Matlab program has been developed to model urethane foaming processes for the purpose of better understanding the foaming process and to advance simulation as a method to develop new foam formulations. As part of the verification of this model, isocyanate reaction profiles were followed for reactions with alcohol, urethane, and epoxy moieties. The isocyanate concentration profiles were consistent with previously published reaction parameters for reactions of isocyanates with alcohols as well as reactions with the urethane moieties formed from reactions with alcohols. The data of this paper indicate that epoxy moieties react directly and indirectly with isocyanates to increase crosslinking. Epoxy moieties were reactive enough to impact temperature profiles during the first few minutes of reaction. Both isocyanate-epoxy and isocyanate-urethane reactions can increase cross-linking during the hours following the initial foaming process.
Methodology which was used for polyurethane study has been expanded to vegetable oil self-polymerization. The vegetable oil reactivity has been analyzed. A model of carbon-carbon double bond reaction between vegetable oil and it copolymer has been established. Reasonable modeling result and theory has been developed. On the topic of the resin polymerization of unsaturated vegetable oils, Chapter 3 presents a summary of the reaction chemistry.