Kinetics of Formation and Gelation Behavior of the Poly (urethane-isocyanurate)

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Abstract

Kinetics of formation of poly(urethane-isocyanurate) (PUIR) from toluene diisocyanate (TDI) and polypropylene glycol (PPG) in presence of dibutyltin dilaurate (DBTDL) was investigated and the kinetic parameters of simultaneous reactions of urethane and isocyanurate formations have been obtained. The gelation behavior of PUIR was studied in the conventional batch reactor as well as in the internal mixer. The results showed that the gelation time can be expressed as a power function of DBTDL concentration. The torque and temperature evolutions were used to present the extent of crosslinking reactions during the formation of PUIR in the internal mixer. The gelation is expedited with increasing r-value, catalyst concentration, temperature and mixing rate. The maximum and final values of torque and temperature, are not so much influenced by catalyst concentration in the mixer. The PUIR samples have been characterized using various measurements.

Keywords - Polyurethane, isocyanurate, kinetics, gelation, internal mixer

INTRODUCTION

Polyurethanes (PU) have been widely used in various industrial applications such as foams, plastics, elastomers and adhesives Isocyanurate-modified polyurethanes poly(urethane-isocyanurate)s (PUIR), are of interest thanks to their good mechanical and physical properties. These polymers have a higher thermal stability and fire resistance than the conventional PUs, due to substituting some urethane groups with more heat-resistance isocyanurate rings, in the chain [1-3]. The two main reactions that lead to formation of urethane and isocyanurate structures are described by following expressions:

Urethane formation:
-NCO + -OH
$$\rightarrow$$
 -NH-CO-O- (1)

In reaction of excess amount of NCO groups of diisocyanates, with OH groups of polyols, both urethane and trimer structures are formed if special kind of catalyst is present. The trimerization of isocyanate groups, eq. (2), results in crosslinking because of tri-functionality of trimers [1,2].

The curing characteristics and thermal flow of thermosetting materials can be evaluated by means of internal mixers. These devices provide useful data to predict the processability of a material in a particular polymer processing [4].