Group Contribution Method to Predict the Flame Resistance of Polycarbonates

Michael Takemori and Moitreyee Sinha, GE Global Research Center, Niskayuna, NY

This presentation documents our recent efforts at modeling and predicting the flame resistance of polycarbonates, related polymers and their copolymers based on their chemical structures. An additivity approach based on group contributions, popularized by van Krevelen, was chosen to be the basis of our structure-property modeling efforts. Recently, Walters and Lyon at the FAA developed a pyrolysis-combustion flow calorimeter (PCFC) to measure the heat release capacity (HRC) of an extensive array of polymers. They related HRC to the flammability of these polymers by showing that it generally correlated with LOI (limiting oxygen index), larger scale flame calorimetry testing and the OSU (Ohio State University) test, an industry standard test protocol. They further demonstrated that HRC, which they called a material fire parameter, could be modeled as the sum of group contributions. Using an extensive HRC database, these researchers computed group contribution values for dozens of distinct structural groups. In our studies, we extended the work of Walters and Lyon to model a large variety of polycarbonate copolymers by adding a few new structural groups and by developing additive group contributions for total heat release and % residual char, two other parameters obtained in the PCFC test. The efficacy of our enhanced model for polycarbonates was demonstrated by successful predictions of copolymer formulations with excellent (PCFC) flammability characteristics.