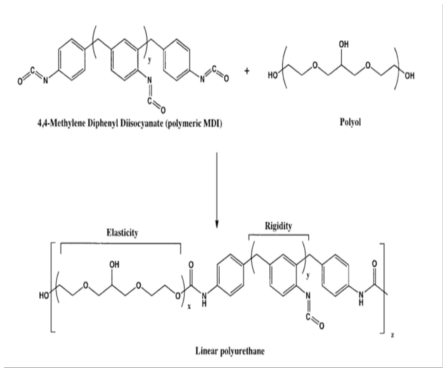
Diffusion Simulation of Flame Retardants in Polyurethane

Jeff Parrozzo and Randall W. Hall
Department of Chemistry
Louisiana State University

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

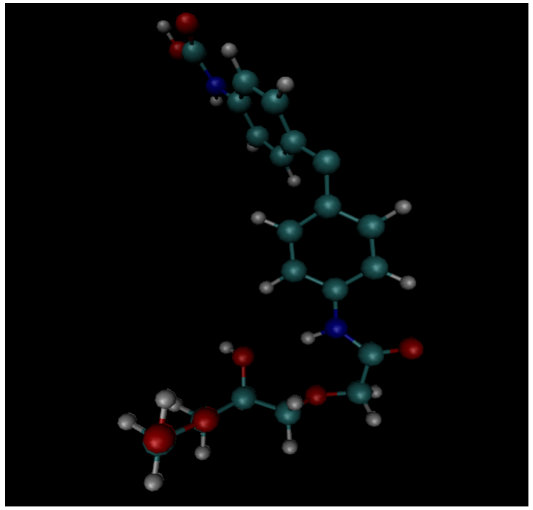
Abstract

Polyurethane is created by reacting two monomers in the presence of a catalyst. The monomers used and the additives introduced during production create different physical properties for different applications. Polyurethane is a widely used polymer with application in everything from insulation foam to automotive parts. The particular type of polyurethane focused on in this research is used primarily in automotive seat cushioning and furniture. The issue with this material is its flammability. Production companies must introduce flame retardants during synthesis in the form of liquids and powders to increase the stability of the polymer. The objective of this research is therefore to determine the conditions under which the flame retardant molecules diffuse into the polyurethane most efficiently. In order to determine this advanced computational tools provided by the LONI supercomputers were utilized for simulation. Although no conclusions were reached, the polyurethane molecule was successfully built and the generation of an environment for the flame retardant molecules to diffuse was near completion.



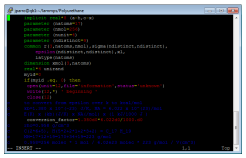
Introduction

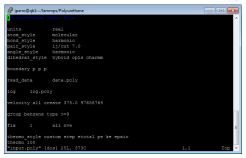
The synthesis of polyurethane involves a step-growth polymerization between a monomer with at least two isocyanate functional groups and another monomer with at least two hydroxyl or alcohol groups in the presence of a catalyst. Different monomers and additives used determines the physical properties of the polyurethane. The particular type of polyurethane analyzed in this research is synthesized by reacting polymeric MDI with a polyol followed by crosslinking with butane diol to create a polyurethane thermoset. Due to the flammability of polyurethane, flame retardants must be introduced during production in the form of liquids and powders. Optimization of the diffusion of the flame retardants thus becomes an important issue. The objective of this research is to determine the best conditions for optimal diffusion of flame retardants in polyurethane. Modeling and simulation was performed on the LONI supercomputers using LAMMPS and visualization with VMD.



Methods

The polyurethane molecule was initially built in Molden in a planar configuration. The structure of the molecule was then optimized on the LONI supercomputers. The LAMMPS script was then written using the z-matrix coordinates from the optimized structure and the force field parameters for each atom type in order to simulate the individual molecule. A fortran code based on Monte Carlo methods was written to replicate the polyurethane molecule and generate an environment for the flame retardant molecules to diffuse.





Future Research

Continuation of this research would require the successful creation of the polyurethane environment for simulation of the diffusion of flame retardant molecule within it. The flame retardant molecules themselves would also need to be created through the same method as the polyurethane molecule.

Acknowledgements

- LA-SiGMA, funded by the National Science Foundation (NSF) award number #EPS-1003897
- Louisiana Optical Network Initiative (LONI)
- Large Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38. (VMD)
- G.Schaftenaar and J.H. Noordik, "Molden: a pre- and post-processing program for molecular and electronic structures", J. Comput.-Aided Mol. Design, 14 (2000) 123-134 (Molden)

LSU