A New Reactive Molecular Dynamics Model for Polymer Pyrolysis

Kenneth D. Smith[a], Stanislav I. Stoliarov[b], Phillip R. Westmoreland[a], Richard E. Lyon[c], and Marc R. Nyden[d], [a] Chemical Engineering Department, University of Massachusetts Amherst, [b] SRA International, Inc., Egg Harbor Twp., NJ, [c] FAA, [d] National Institute of Standards and Technology, Gaithersburg, MD.

We have developed an extension of classical force-field-based molecular dynamics (MD) to the simulation of chemical reactions. Our new Reactive Molecular Dynamics approach called RxnMD is implemented using potential energy surfaces of chemical reactions that are constructed from functions and parameters of a traditional (non-reactive) force field. The method is being designed to model pre-defined reaction types accurately by smoothly interpolating between non-reactive potential energy terms describing reactants, transition state, and products. The objective of this method is to understand polymer flammability and to guide future polymer synthesis.