

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

High-temperature thermal degradation of polyethylene from reactive molecular dynamics J. MATTHEW D. LANE, NATHAN W. MOORE, Sandia Natl Labs — Thermal degradation of polyethylene is studied under extremely high-rate temperature ramp rates from 10^{14} to 10^{10} K/s in isochoric, condensed phases. The molecular evolution and macroscopic state variables are extracted as a function of density from reactive molecular dynamics simulations using the ReaxFF potential. These results are used to parameterize a kinetic rate model for the dissociation and coalescence of hydrocarbons as a function of temperature, temperature ramp rate, and density. The results are contrasted to first-order random-scission macrokinetic models often assumed for pyrolysis of linear polyethylene under ambient conditions. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04- 94AL85000.

J Matthew Lane
Sandia Natl Labs

Date submitted: 06 Nov 2015

Electronic form version 1.4