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Mega-supramolecules for safer, cleaner fuel

JULIE KORNFIELD, Invited Speaker

Guided by the statistical mechanics of ring-chain equilibrium, we designed and synthesized polymers that self-assemble into "mega-supramolecules" ($\geq$5,000 kg/mol) at low concentration ($\leq$0.3%wt) in hydrocarbon liquids. Experimental results accord with model predictions that end-functional polymers, which distribute among cyclic and linear supramolecules, can form a significant population of mega-supramolecules at low total polymer concentration—if, and only if, the backbones are long (>400 kg/mol) and end-association strength is optimal (16-18kT). Hydrocarbon liquid fuels are the world's dominant power source (34% of global energy consumption). Transportation relies heavily on such liquids, presenting the risk of explosive post-impact fires. The collapse of the World Trade Center on September 11, 2001 inspired us to revisit polymers for mist control to mitigate post-impact fuel explosions. Rheological and both light and neutron scattering measurements of long end-functional polymers having polycyclooctadiene backbones and acid or amine end groups verify formation of mega-supramolecules. Post-impact flame propagations experiments show that mega-supramolecules control misting. Turbulent flow measurements show that mega-supramolecules reduce drag like ultra-long covalent polymers. With individual building blocks short enough to avoid hydrodynamic chain scission (400<M_w [kg/mol] $\leq$1,000) and reversible linkages that protect covalent bonds, they respond reversibly to flow through pumps and filters without degradation. Mega-supramolecules had no adverse effect on power output, fuel efficiency or emissions in diesel engines. In fact, they gave a 12% reduction in diesel soot. Thus, long end-associative polymers may open the way to fuel additives that reduce pollution and improve transportation safety and security.