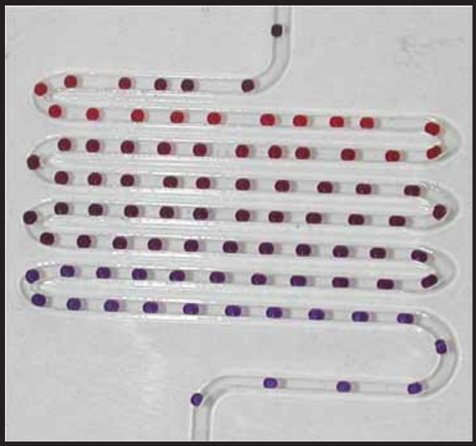
Sustainable Polymers

Objective



Our goal is to deliver measurements and methods that enable an increase in production and diversification of bio-based, renewable soft materials and reduce the impact of petroleum-based materials manufacturing on the environment.

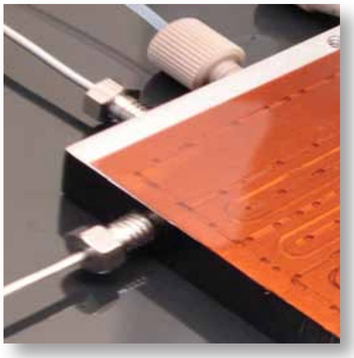
These materials will have the performance and functionality to enable replacement or improvement of current materials with the confidence that their environmental impact is minimized and quantified.

Impact and Customers

- 3.4% of US Petroleum Consumption is dedicated to chemical, plastic and rubber products with an estimated value added of $375 Billion
- The current petroleum-based materials industry is based on a foundation of classical transformations exploiting carbon-carbon bond formation and breaking, often using heavy metals, and decades of development in separations by distillation for feedstock refinement.
- To accelerate the production and use of renewable materials, substantially different measurement methods and standards are needed. New processing routes require a paradigm shift that includes expanded exploitation of heteroatom bonds, biological catalysis pathways (in vitro enzymes and fermentation) and separation technologies based on extractions.

- We will develop the measurement tools needed to establish the relationships between the chemistry, structure and composition of novel materials fabricated from bio-based feedstocks, and their performance and degradation behavior.
- Customers range from manufacturers of construction materials to developers of sophisticated technological applications of soft materials in the areas of nanotechnology and renewable energy and transportation.

Approach



Renewable materials present a different set of characterization challenges. A balanced perspective that considers the value of and measures the extent of desirable degradation will provide industry with the coveted tools they need to evaluate long-term environmental impact, while maintaining or exceeding existing performance metrics.

This general approach is rooted in our experience with combinatorial method development, organic polymer synthesis, and microfluidic devices for applications in polymer science. We will integrate state-of-the-art analytical tools such as Matrix Assisted Laser Desorption Ionization Mass Spectrometry (MALDI-MS) and advanced Nuclear Magnetic Resonance techniques to understand composition and functionality of polymers produced using green transformation routes and renewable monomer sources. The effort will be coordinated with colleagues with expertise in thin film adhesion and mechanics, and composite and fiber testing.

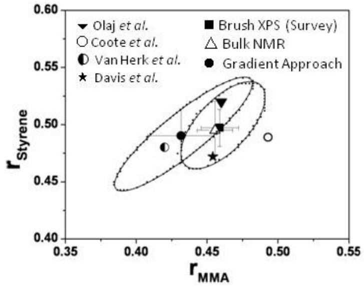
POLYMERS

Accomplishments

Background
Interest in renewable materials stems from the desire to reduce the use of petroleum-based materials, and thereby reduce the energy consumption and environmental emissions associated with production, as well as eliminate reliance on unsustainable chemistry and processing routes that use toxic reagents and precious, non-renewable resources. Furthermore, increasing renewable content is often correlated to increased degradability, enabling elimination of many materials from waste streams and reducing long ecosystem residence times.

The pipeline of renewable material candidates, derived from bio-based feedstocks, has been slowed by challenges in the discovery and optimization of transformation routes, development and processing of new materials, and the assessment and test method development of new performance metrics that incorporate sustainability principles. Without a strong technical foundation and transformational scientific advances, it is unclear whether products from bio-based renewable feedstocks can compete economically with those from petroleum-based feedstocks, and respond to new consumer demands in the production of chemicals and materials.

To meet these challenges, substantial gains in basic control of processes, from refinement to processing and production are critical. Beyond the market, security and climate drivers, there are environmental benefits to the use of bio-based feedstocks, including reduced consumption of natural resources and increased safety.



Reactivity Ratios for Styrene Methyl Methacrylate Polymerizations measured from a copolymer library fabricated in a microchannel

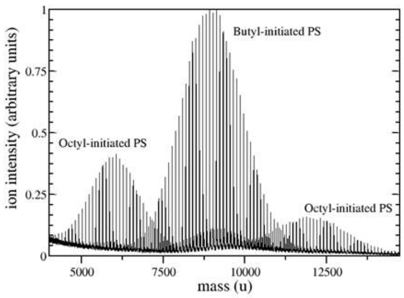
Microfluidic Polymerizations
Efforts in the Sustainable Polymers Project at NIST will focus on developing microfluidic and other methods to characterize in vitro and in vivo enzymatic tranformation routes to create polymers from multiple monomer feedstocks, ultimately focusing on the incorporation of higher renewable monomer content in polymeric materials with a high level of control in molecular architecture and functionality.

Research in the NIST Combinatorial Methods Center has applied microfluidic devices to characterize block and statistical copolymerizations using conventional and controlled radical polymerizations, and living anionic polymerizations. Combining libraries of materials prepared at the microscale with analytical tools such as Raman spectroscopy and X-ray photoelectron spectroscopy, characteristics of the polymerizations (extent of reaction, reactivity ratios) were measured.

Capabilities that have been developed as a part of this program include polymerizations in continuous flows, droplets and on surfaces enabling flexible reaction environments. This work has been disseminated via technical publications, presentations at workshops, national and international meetings, and collaborations with Rhodia and BASF.

Precision control and rapid tuning enabled by the microscale reaction environment will enable similar measurements of polyester and other polymerizations via enzyme catalysis rather than transition metals. The fundamental insights provided by these measurements will enable broader utility and advanced applications of these green reactions.

Advanced molecular characterization
Our expertise in the use of state-of-the-art analytical techniques such as Matrix Assisted Laser Desoprtion/Ionization Mass spectrometry (MALDI-MS) has enabled characterization of chain architecture, polydispersity and end group analysis. These techniques and other complimentary tools will be applied to improve understanding and control of copolymerization behavior in the same material libraries prepared in microfluidic devices.



MALDI-MS data for a mixture of end-group functionalized polystyrenes

Learn More

William Wallace
Kathleen Flynn

Kathryn Beers
(Polymers Division)
(301) 975-2113
beers@nist.gov
www.nist.gov/polymers

Publications

Iida K, Chastek TQ, Beers KL, Cavicchi KA, Chuna J and Fasolka MJ *Living Anionic Polymerization Using a Microfluidic Reactor* Lab Chip, 8:950 (2008)

Patton DL, Page KA, Xu C, Genson KL, Fasolka MJ and Beers KL *Reactivity Ratios in Surface-Initiated Copolymerization* Macromolecules, 40: 6017 (2007)

Wallace WE, Guttman CM, Flynn KM and Kearsley AJ *Numerical Optimization of Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry: Application to Synthetic Polymer Molecular Mass Distribution Measurement* Analytica Chimica Acta, 604:72 (2007)

Barnes SE, Cygan ZT, Yates JK, Beers KL and Amis EJ *Raman Spectroscopic Monitoring of Droplet Polymerization in a Microfluidic Device* The Analyst, 131:1027 (2006)

Wu T, Mei Y, Cabral JT, Xu C and Beers KL *A New Synthetic Method for Controlled Polymerization Using a Microfluidic System* J. Am. Chem. Soc., 126:7880 (2004)