UNIVERSITY OF DELAWARE

CENTER FOR PLASTICS INNOVATION at the UNIVERSITY OF DELAWARE

THRUST 3

CPI develops new cross-cutting tools driven by artificial intelligence, plastics waste characterization, macromolecular property prediction, and additive manufacturing to enable scientific advances.

CHALLENGES

Developing and evaluating new processes to valorize plastics waste can be arduous due to the diversity of feedstock, processing challenges inherent to large polymer molecules, characterization of products, and quantification of the impact/economics.

COMPLEX MIXTURES

Plastics are an intricate mixture of various macromolecules and small molecule additives

POLYMER MELT

The polymer melt during deconstruction is complex and evolves during the process

VISCOSITY and CONDUCTIVITY

Processes are challenged by the high viscosity and low thermal conductivity of polymers

SCATTERED DATA

Relevant data are scattered and difficult to utilize for new materials/methods

VALORIZATION APPROACHES

Valorization approaches can lead to diverse products and need quantification of impact

OUR GOALS

CHARACTERIZE

Characterize the effects of 'real' plastics (mixture of polymers with various architectures and additives) on valorization processes and resulting products

PREDICT

Predict macromolecular properties relevant to plastics waste deconstruction processes through modeling

DEVELOP

Develop automated software tools to extract plastics upcycling/ recycling information from literature

CREATE

Create approaches to additive manufacturing to produce plastics designed for more efficient upcycling/ recycling

QUANTIFY

Quantify valorization processes using Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA)

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COMPUTATIONAL TOOLS

NATURAL LANGUAGE PROCESSING

Algorithms search literature on research topics related to plastics waste recycling/upcycling materials and processes, extract targeted information, and help researchers utilize this knowledge toward new research directions. These tools can crawl millions of scientific articles and enable efficient data annotations for machine learning algorithms.

FIRST PRINCIPLES MODELING

Multi-scale modeling of macromolecular transformations on supported catalysts and inside porous materials simulate the reaction of the macromolecule at the active site of the catalyst. These calculations are essential to understand and provide insight into catalytic processes.

ATOMISTIC and COARSE-GRAINED SIMULATIONS

Molecular dynamics and Monte Carlo simulations investigate polymer blends, polymers in catalyst pores, and preferential adsorption. This includes modeling the transport of polymers in catalyst pores by examining the effect of cylindrical nanoconfinement as well as interfacial behavior of polymers at pore surfaces.

MACHINE LEARNING REGRESSION MODELS

Integrated with molecular dynamics calculations, models predict thermodynamic and transport properties of polyolefin blends at concentrations, temperatures, and pressures relevant to upcycling processes. Structure-property relations of polyethylene-like materials are modeled for sustainable polymer design.

LIFE CYCLE ASSESSMENT, TECHO-ECONOMIC ANALYSIS

Models and calculations quantify the environmental and economic impacts of novel valorization processes. Uses include benchmarking against incumbent technologies, sensitivity analyses around process inputs, and scale-up from laboratory results.

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EXPERIMENTAL TOOLS

'REAL' PLASTICS CHARACTERIZATION

Established approaches study the complex nature of plastics waste including the effects from additives, contaminants, polymer molecular weight, and macromolecular architecture on valorization routes. The experimental protocols and data analysis practices facilitate expansion of processes to accommodate feedstock variability.

MICROWAVE REACTORS

Microwave heating of a polymer, catalyst, and microwave susceptor slurry offers an opportunity to overcome the low thermal conductivity of polymers, speed up polymer valorization processes, and lower energy requirements for polymer deconstruction. Capabilities include a custom high precision microwave reactor with in-situ analytical capabilities.

ADDITIVE MANUFACTURING TECHNIQUES

A patent-pending extruder design enables 3D printing of objects from a pellet or powder feedstock rather than relying on traditional polymer filaments. This advancement expands the portfolio of polymeric materials that can be readily 3D printed as well as more easily allows inclusion of recycled plastics waste into products.

HIGH-THROUGHPUT CATALYSIS INVESTIGATIONS

In collaboration with the High Throughput Experimentation (HTE) Center at the University of Delaware, a multi-cell reactor was developed to withstand the high temperatures and pressures associated with polymer deconstruction experiments. This capability allows for fast screening of catalysts, reaction conditions, or feedstocks.

VALORIZATION PRODUCT ANALYSIS

Analytical approaches connect traditional polymer characterization techniques and mechanistic insights to target high-value products from novel valorization processes. Quantitative methods evaluate valorization products with a broad distribution of characteristics, particularly molecular weight, and provide critical feedback for process optimization and mechanistic insights.

PUBLICATION HIGHLIGHTS

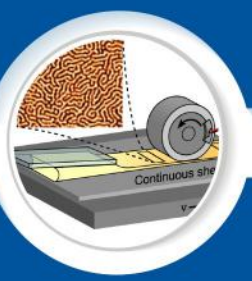
Journal of Chemical Information and Modeling (2022)

UNLEASHING POWER OF KNOWLEDGE EXTRACTION FROM SCIENTIFIC LITERATURE IN CATALYSIS

Green Chemistry (2022)

ANTIOXIDANT INDUCED TRANSFORMATIONS OF A METAL-ACID HYDROCRACKING CATALYST IN THE DECONSTRUCTION OF POLYETHYLENE WASTE

ACS Applied Polymer Materials (2022)



INLINE ROLLING SHEAR ALIGNMENT: LONG-RANGE ORDER OF BLOCK POLYMER VIA A FAST, CONTINUOUS, SINGLE-STEP PROCESS

Annual Review of Materials Research (2022)

INNOVATIONS TOWARD THE VALORIZATION OF PLASTICS WASTE

ACS Catalysis (2023)

COMPUTATIONAL INVESTIGATION OF SITE-DEPENDENT ACTIVATION BARRIERS OF ZEOLITE-CATALYZED PROTOLYTIC CRACKING REACTIONS

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