U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Automatic Monitoring & Control of Polymer Reactions — Development and Implementation of an Automatic Continuous Online Monitoring and Control Platform for Polymerization Reactions

Figure 1. Researchers developed basic control and automation technology using the laboratory scale Automatic Continuous Online Monitoring of Polymerization reactions/ Control Interface (ACOMP/CI) system. The technology was validated using the ACOMP/CI pilot system with 64L reactor shown above. *Photo credit Tulane.*

Enabling energy and resource efficiency in polymer manufacturing

Polymers, such as plastics, are an important class of chemical compounds composed of many repeated sub-units of monomers. The ability to engineer them to yield a desired set of proper- ties (strength, stiffness, density, heat resistance, electrical conductivity) has greatly expanded the many roles they play in the modern industrial economy.

Market applications of polymers include composite building materials, paints, adhesives, coatings, personal care products, biomedical components, and ‘intelligent’ new materials.

Despite the important role of polymers, due to the complexity of characterizing polymers, the design and implementation of polymer reactors is still an art rather than a science relying on operator judgment and reaction ‘recipes.’ Most polymer processes utilize time-consuming and labor-intensive offline analyses to validate, perform quality control, and provide some level of process control. Major problems can also occur during reactions, for example, runaway and dangerously exothermic reactions, failed reactions, production of unwanted side products, and reactor fouling. As a result, polymer production is highly inefficient with high levels of product waste and lost production time.

This project targeted inefficiencies to enhance sustainability of polymer production by creating a paradigm shift in the way polymers are manufactured. Researchers used an existing platform called the Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP) developed and patented at Tulane University. This system relies on continuous sample withdrawal, dilution, conditioning, and measurement to provide data on multiple critical polymer properties; reaction monitoring with ACOMP at lab, pilot, and industrial scales was previously validated.

Researchers developed predictive models driven by this data and integrated modeling and automated feedback control to create the ACOMP/Control Interface (or ACOMP/CI).

Benefits for Our Industry and Our Nation

The ACOMP/CI platform is fully compatible with current polymer manufacturing infrastructure and will enable:

- Increased production efficiency due to a reduction in grade changeover time, off-spec production, and unexpected production events.
- Increased efficiency by following optimized reaction trajectories during manufacture.
- Reduced energy and material feedstock consumption per pound of polymer produced.

Applications in Our Nation’s Industry

While the ACOMP/CI platform is developed specifically for polymerization reactions, the impact could be significant since the market applications of polymers are extremely broad. The polymer industry provides materials for sectors such as automotive, aerospace, agriculture, paints, resins, adhesives, optics, electronics, lightweight building materials, and many more. The ACOMP/ CI system should also enable more efficient development of new and better polymers for ‘intelligent’ new materials.

Project Description

This project used Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP), integrated for the first time with modeling and feedback control to create the innovative ACOMP/ CI. At the completion of the project, ACOMP/CI was a self-contained intelligent system for advanced operation and control of polymerization processes that can be used throughout the polymer industry.

Barriers

- Establishing polymerization reaction process characteristics that are broadly applicable across the polymer industry to enable feedback control.
- Designing and implementing a reliable ACOMP/CI prototype for the industrial environment.

Pathways

Conceptual feasibility was demonstrated by reaction control on simple free radical polymerization reactions. The early phase data was used to design and build an ACOMP/CI system comprised of a pilot reactor, the ACOMP system and the control interface. Initially the ACOMP/CI system was challenged to follow specified, well understood reaction trajectories using manual active control. Manual active control allows an operator to 'drive' the monitored reaction as close to an ideal polymerization reaction trajectory as possible.

A matrix of industrially relevant reactions was developed and the reaction characteristics within ACOMP/CI control capabilities were established. Advanced model-based control and monitoring algorithms were developed based on these reactions. Automatic feedback control was tested and validated by achieving desired reaction trajectories and final polymeric products (Figure 2). Software modules were developed and finalized into reliable, automated, working code for a commercial prototype to ensure accelerated commercialization and industrial implementation.

Milestones

This two year project started in December 2014 and was completed in 2017.

- Design and build of a high performance, versatile pilot reactor outfitted with ACOMP and CI, and parallel design and build of an industrial prototype at the IIP facility (Completed).

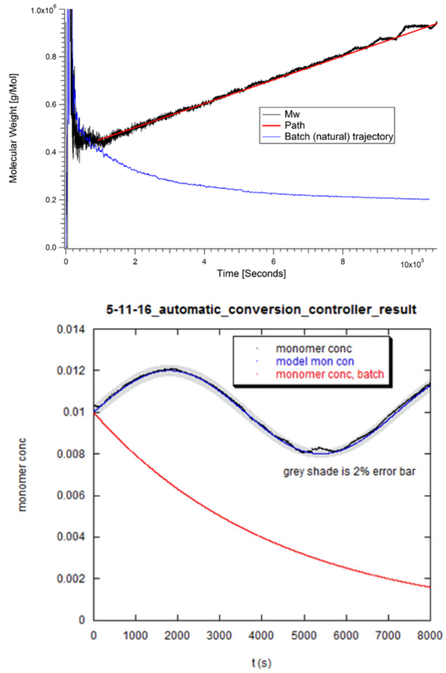

Figure 2. First ever automatic feedback control of molecular weight during polymerization, top, shows linearly increasing target Mw trajectory (red), and the reaction that followed it (black). Automatic control of conversion (black) along a sinusoidal target trajectory (blue) is shown in the bottom graph

- Demonstrate manual active control of the ACOMP/CI at full pilot scale by steering an acrylamide homopolymerization reaction along a pre-determined trajectory (Completed).
- Demonstrate ACOMP/CI control at pilot scale of a selected matrix of industrially relevant polymerization reactions (Completed).
- Develop advanced model-based control and data-driven non-linear monitoring algorithms and deploy for reaction control on the ACOMP/CI (Completed).

Accomplishments

- Designed, implemented, and tested an open source platform that allows full functionality and connectivity to update and modify polymer process behavior in the existing ACOMP system.
- Visualization and modification of control parameters while a reaction progresses is enabled through a user-friendly graphic user interface.

Technology Transition

Researchers are actively engaged in promoting the new technology to potential customers. Fluence Analytics, the project's commercialization partner, is working with a client to deliver a prototype control interface software package for the client's ACOMP system. The client has very tight specifications for their product and hopes to optimize their manufacturing process and consistently improve product quality with the controller. Fluence is also negotiating with several other polymer manufacturers for ACOMP installation and the possibility of extending to ACOMP/CI. Researchers are seeking further funding to develop ACOMP/CI for polyolefins, a sector with potentially the greatest energy savings and waste reduction.

Project Partners

Tulane University
New Orleans, LA
Principal Investigator: Wayne Reed
Email: *wreed@tulane.edu*

Fluence Analytics (formerly Advanced Polymer Monitoring Technologies, LLC)
New Orleans, LA

Louisiana State University
Baton Rouge, LA

For additional information, please contact

Dickson Ozokwelu
U.S. Department of Energy
Advanced Manufacturing Office
Phone: (720) 356-1754
Email: *Dickson.Ozokwelu@ee.doe.gov*

Project final report available at
www.osti.gov/scitech:
OSTI Identifier 1399518

U.S. DEPARTMENT OF ENERGY
Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

For more information, visit:
energy.gov/eere/amo

DOE/EE-1681 · October 2018