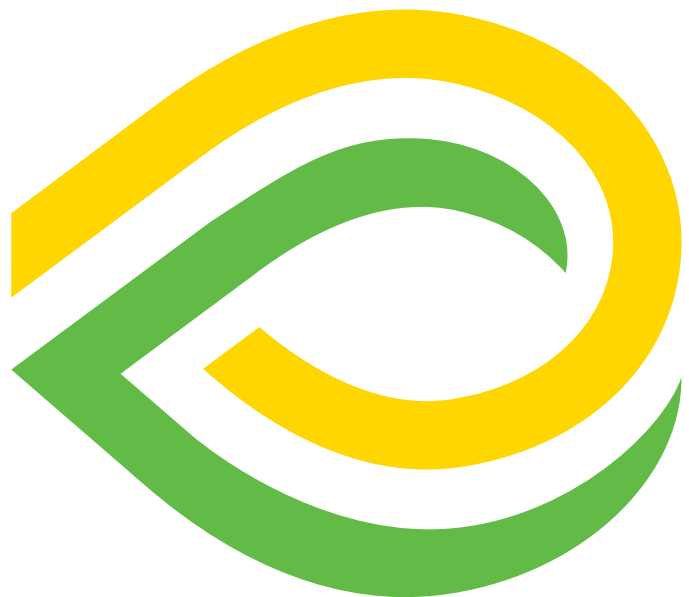


U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Annual Review of Research
FY 2022



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List of Acronyms

BETO	Bioenergy Technologies Office
CFP	catalytic fast pyrolysis
CMA	critical material attribute
DEM	discrete element method
DMR	deacetylation and mechanical refining
FAIR	findable, accessible, interoperable, and reusable
FCIC	Feedstock-Conversion Interface Consortium
FY	fiscal year
LCA	life cycle analysis
MRF	material recovery facility
MSW	municipal solid waste
QbD	quality by design
SAF	sustainable aviation fuel
TEA	techno-economic analysis

Executive Summary

The Feedstock-Conversion Interface Consortium (FCIC) develops first-principles-based knowledge and tools to understand, quantify, and mitigate the effects of feedstock and process variability across the bioenergy value chain, from the field and forest through downstream conversion. The FCIC is a collaborative and coordinated effort involving researchers in many different disciplines. It is led by the U.S. Department of Energy's Bioenergy Technologies Office and includes researchers from nine national laboratories: Argonne National Laboratory, Idaho National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Energy Technology Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories.

Research within the FCIC focuses on two complementary conversion pathways: (1) the low-temperature conversion of corn stover to fuels and chemicals using deacetylation and mechanical refining, enzymatic hydrolysis, and biological upgrading of the sugar- and lignin-rich streams; and (2) the high-temperature conversion of pine residues to fuels using catalytic fast pyrolysis and hydrotreating. Each pathway covers three sequential process areas—biomass harvest and storage, preprocessing, and conversion. In Fiscal Year (FY) 2022, FCIC researchers added municipal solid waste as a nontraditional but low-cost feedstock. The preliminary work in this area focused on the characterization of landfill-bound residues from a recycling facility, also referred to as a material recovery facility.

The FCIC is organized into eight collaborative tasks working in each of these process areas. The Feedstock Variability task investigates biomass attribute variations that originate in the beginning of the overall bioenergy value chain; the Preprocessing, Materials Handling, and Materials of Construction tasks investigate the effects of biomass variability in the preprocessing area; and the High-Temperature Conversion and Low-Temperature Conversion tasks investigate the effects of biomass variability in the conversion process area. Two supporting tasks (Crosscutting Analyses and Scientific Data Management) support all FCIC research.

This is the third annual report from the FCIC and presents an overview of the research accomplishments of FCIC members in FY 2022, covering both the low- and high-temperature conversion pathways and all three process areas (feedstock harvest and storage, preprocessing, and conversion). The key research achievements of each task are presented, along with planned FY 2023 work that will build on the accomplishments of FY 2022.



The Feedstock-Conversion Interface Consortium uses first-principles-based science to de-risk biorefinery scale-up and deployment by understanding and mitigating the impacts of feedstock variability on bioenergy conversion processes.

energy.gov/fcic

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Introduction and Background

The Feedstock-Conversion Interface Consortium (FCIC) uses first-principles-based science to de-risk biorefinery scale-up and deployment by understanding and mitigating the impacts of feedstock variability on bioenergy conversion processes. FCIC researchers are developing knowledge to provide bioenergy industry stakeholders a fundamental understanding of the variability in the chemical, physical, and mechanical properties of biomass feedstocks and process intermediates based firmly on first-principles science, as well as tools to assess and mitigate the impact of this variability on the performance of the overall system.

Feedstocks and Conversion Pathways

Research within the FCIC is focused on two complementary conversion pathways: (1) the low-temperature conversion of corn stover to fuels and chemicals using deacetylation and mechanical refining (DMR), enzymatic hydrolysis, and biological upgrading of the sugar- and lignin-rich streams; and (2) the high-temperature conversion of pine residues to fuels using catalytic fast pyrolysis (CFP) and hydrotreating. Both pathways are being investigated by core Bioenergy Technologies Office (BETO) projects, and thus the FCIC complements existing BETO efforts, focusing on the impacts of feedstock and process variability.

In Fiscal Year (FY) 2022, FCIC researchers expanded the feedstocks being investigated to include municipal solid waste (MSW). Using MSW as a low-cost feedstock will present challenges across the bioenergy value chain, including handling, preprocessing, and conversion. Because MSW is a diverse category, encompassing everything from food waste to potentially recyclable material, we began this work by focusing on the landfill-bound material from a material recovery facility (MRF). These MRF residues comprised both cellulosic (e.g., cardboard, office paper, newsprint) and plastic materials.

FCIC Organization

The FCIC is a collaborative and coordinated effort involving research teams representing nine national laboratories: Argonne National Laboratory, Idaho National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Energy Technology Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories.

The FCIC is organized into eight collaborative tasks working in each of the three process areas (Figure 1). The Feedstock Variability task is investigating attribute variations that originate from environmental factors and supply chain operations in the harvest and storage process area; the Preprocessing, Materials Handling, and Materials of Construction tasks are investigating the preprocessing area; and the High-Temperature Conversion and Low-Temperature Conversion tasks are investigating the conversion process area. Two enabling tasks (Crosscutting Analyses and Scientific Data Management) support all FCIC research. To understand the economic impacts of the knowledge and tools being developed by the FCIC, the Crosscutting Analyses task leverages detailed techno-economic analysis (TEA) and life cycle analysis (LCA) modeling approaches (developed over the course of many years under core BETO research projects) to perform targeted case studies, which will provide high-level cost–benefit analyses to quantify the economic impacts of FCIC research. The Scientific Data Management task is using a centralized scientific data management system to ensure that the underlying data generated by the various research groups and used to test hypotheses regarding the impacts of feedstock and process variability will be widely available.

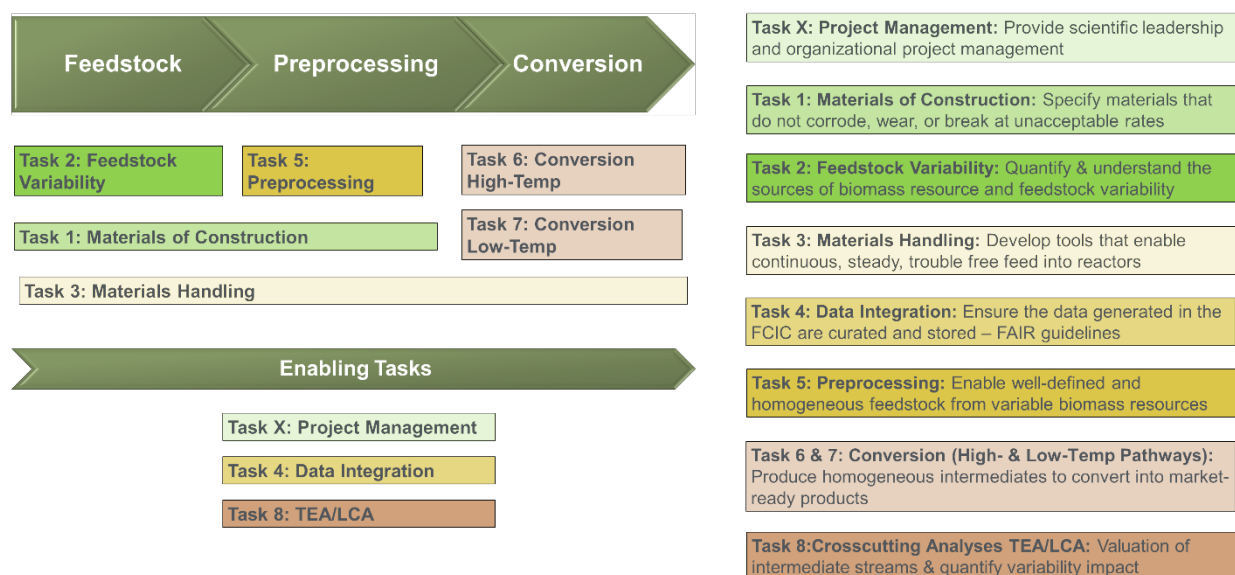


Figure 1. FCIC tasks span the entire bioenergy value chain: feedstock, preprocessing, and conversion.

Quality by Design

The overall technical approach of the FCIC is based on the “quality by design” (QbD) concept, originally developed by Dr. Joseph M. Juran.¹ QbD has been embraced by manufacturers across the globe and has also been adopted by the U.S. Food and Drug Administration,² which oversees pharmaceutical manufacturing in the United States. QbD is consistent with the concepts of “total quality management” and “continuous quality improvement,” which have revolutionized the way products are manufactured over the last several decades.

FCIC researchers are adapting QbD principles to their research efforts. They are emphasizing a number of key elements of the QbD approach, including (1) developing a comprehensive understanding of unit operations based on fundamental science, (2) focusing work on individual unit operations within the overall bioenergy value chain, and (3) investigating the behavior of these unit operations in terms of their inputs (referred to as critical material attributes [CMAs]), their outputs (critical quality attributes), and their operational parameters (critical process parameters). Figure 2 shows a schematic overview of the relationships among these inputs, outputs, and operational parameters within the QbD framework.

¹ J. M. Juran. 1992. *Juran on Quality by Design: The New Steps for Planning Quality into Goods and Services*. New York: Free Press.

² U.S. Food and Drug Administration. 2007. *Pharmaceutical Quality for the 21st Century: A Risk-Based Approach Progress Report*. Washington, D.C.: FDA. www.fda.gov/about-fda/center-drug-evaluation-and-research-cder/pharmaceutical-quality-21st-century-risk-based-approach-progress-report.

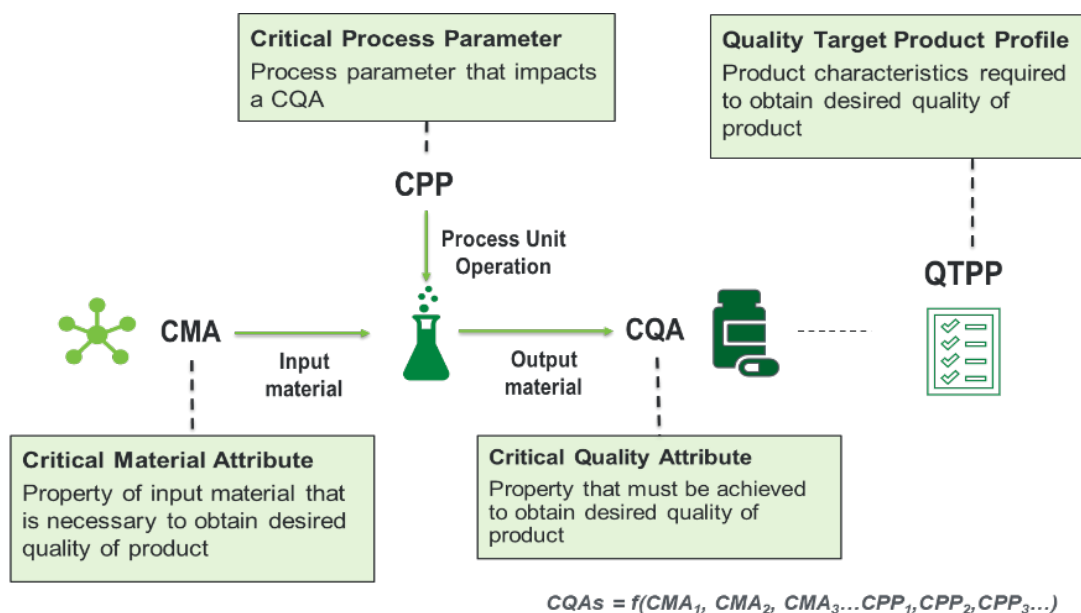


Figure 2. QbD parameter names and descriptions

Task Accomplishments

This report presents a high-level overview of the accomplishments of the FCIC in FY 2022, covering both the low- and high-temperature conversion pathways and all three process areas (feedstock harvest and storage, preprocessing, and conversion). The key research achievements of each task are presented, along with planned FY 2023 work that will build on the FY 2022 accomplishments. A full list of publications is available on the FCIC website: www.energy.gov/eere/bioenergy/fcic-publications.

Task 1 – Materials of Construction

The Materials of Construction task uses integrated efforts of characterization, modeling, and testing to (1) gain a fundamental understanding of failure modes and wear mechanisms, (2) develop analytical tools to predict wear and establish material properties, (3) select and evaluate candidate approaches to mitigate wear, and (4) share the knowledge and wear mitigation strategies with the biomass industry. The knowledge and tools developed here will enable the rapid design and selection of materials that resist wear and maintain structural integrity, resulting in sustainable performance and improved product quality.

FY 2022 Key Results

Laboratory-Scale Testing of MSW Abrasiveness

Task 1 researchers added an additional tool for measuring the abrasiveness of MSW materials. By modifying a well-accepted standard abrasion test from ASTM International,³ Task 1 researchers developed a laboratory-scale tool for characterizing MSW materials. The tool will permit the rapid, cost-effective characterization of abrasiveness of MSW materials to either rank the abrasive wear resistance of potential wear mitigation strategies (e.g., surface coatings, advanced materials) or rank the abrasiveness of different MSW samples.



Figure 3. Laboratory-scale equipment to rapidly characterize MSW abrasiveness using a method based on an ASTM-approved test standard (G65)

TEA of Knife Mill Blades

Task 1 researchers completed small-scale experiments to characterize the wear behavior of biomass comminution using a knife mill, determining the wear behavior of blades made of standard M2 steel (the default case), as well as M2 steel blades with a

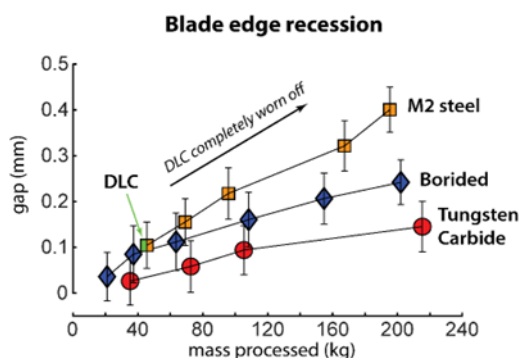


Figure 4. Reduced rates of blade edge recession led to longer lifetimes and more favorable economics.

surface coating of iron boride (FeB) and blades made of tungsten carbide (WC). This work demonstrated a modest positive internal rate of return of knife mill operation due to the longer life of either the FeB-coated or WC blades. The Task 1 researchers shared the wear information with Task 8 researchers, who then used a discrete event simulation model of the overall biorefinery to estimate the impact of more durable blades on biorefinery performance. The reduced mill downtime associated with either the FeB-coated or WC blades resulted in increased overall biomass feedstock throughput, dramatically increasing the internal rate of return of either advanced wear mitigation strategy. The researchers are in the process of publishing this TEA in a peer-reviewed journal article.

FY 2023 Goals

In FY 2023, Task 1 researchers will continue their work to conduct a TEA for the improved economics by using wear-resistant tools for knife milling, refine the analytical wear models, develop characterization and testing protocols for assessing MSW abrasiveness, and identify additional wear-prone comminution or handling devices used for biomass or MSW preprocessing. This work will focus on understanding the key components in MSW samples that drive equipment wear, and using the knowledge gained in addressing wear issues caused by biomass feedstocks to investigate wear in MSW processing equipment.

³ ASTM International. 2021. "ASTM Standard G65, Standard Test Method for Measuring Abrasion Using the Dry Sand/Rubber Wheel Apparatus."

Task 2 – Feedstock Variability

The Feedstock Variability task aims to identify and quantify the initial distribution of feedstock material attributes and to inform strategies to reduce and manage this variability. Understanding the sources of biomass variability from biomass feedstock harvest and storage operations (e.g., growth conditions, harvest conditions, degradation during storage) will enable the identification and quantification of material attribute variability. Task 2 researchers work closely with other FCIC researchers to share their fundamental learnings on feedstock variability's magnitude and potential impacts across the bioenergy value chain.

FY 2022 Key Results

Drought-Impacted Corn Stover

FCIC researchers are investigating the impact of drought on the physical, chemical, and mechanical attributes of corn stover, and the implications of these impacts on corn stover preprocessing, pretreatment, and conversion. Task 2 researchers led the characterization efforts for two corn stover samples, both harvested from the same location but in two different years, with one harvest experiencing a drought event late in the growing season and one with average precipitation throughout the growing season. Substantial differences were seen in the relative amounts of anatomical fractions, with drought-impacted corn stover having much smaller amounts of cob and husk. However, no major differences were seen in the chemical composition of the individual anatomical fractions between harvest years, and the results of multiple characterization methods used to quantify differences in the structural and mechanical attributes have not yet shown large drought impacts. Experiments are underway to determine conversion performance differences.

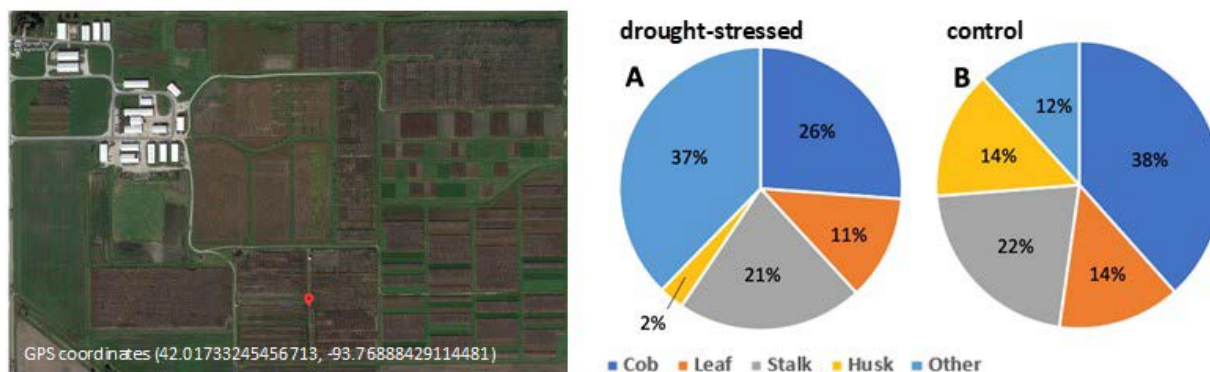


Figure 5. Characterizing the physical, chemical, and mechanical properties of corn stover samples harvested from the same location in both normal and drought years will help elucidate the impact of drought on biomass variability.

Cell Wall Architecture Impacts Deconstruction Modes

Task 2 researchers developed and implemented methods to interrogate the structural integrity of biomass particles at the tissue, cellular, and cell wall scales using optical microscopy and scanning electron microscopy to identify fracture points during simulated comminution experiments. They found that tissues with weak cell-to-cell adhesion will tend to fracture between cell walls, while tissues with strong cell-to-cell adhesions appear to have an equal mix of fractionation between and through cell walls. These findings suggest that comminution behavior originates at the tissue scale and that physical and mechanical attributes at the tissue scale may influence comminution and downstream chemical conversion performance.

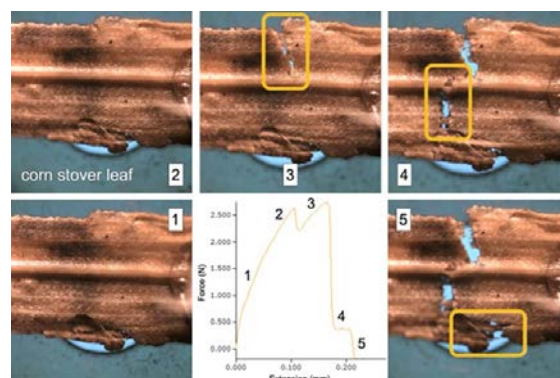


Figure 6. Optical micrographs show how a corn stover leaf loses structural integrity as force is applied.

Image Analysis for Rapid Assessment of Corn Stover

Because of the intrinsic heterogeneity of biomass feedstocks, the material attributes of specific biomass feedstock lots can vary widely, making it difficult to ascertain the value of a particular lot accurately. Low-cost, rapid characterization of the material attributes of specific biomass lots continues to challenge bioenergy stakeholders. Task 2 researchers investigated correlations between low-cost images of corn stover samples and their chemical and mechanical attributes to address this challenge.⁴ The researchers used standard image analysis techniques to extract features from red-green-blue (RGB) color space to investigate variations in CMAs from the chemical composition of corn stover. They showed correlations between the red band intensity and biomass composition and the extent of biological degradation. While preliminary, this work suggests that farmers could use low-cost images for in-field assessment of biomass quality, or that biorefinery operators could use them for online, real-time process control.



Figure 7. Image analysis tools can help screen and classify biological degradation and soil contamination in corn stover.

FY 2023 Goals

In FY 2023, Task 2 researchers will continue their efforts to characterize intrinsic variability in the chemical, physical, and mechanical properties of biomass feedstocks and to understand (in collaboration with other FCIC researchers) how this intrinsic variability affects downstream unit operations. They will also be applying their characterization tools to representative MSW samples. Finally, they will share some of the learnings of their investigations in industry trade journals, providing suggestions for minimizing biomass variability due to biological degradation.

⁴ L. Ding, A.N. Hoover, R.M. Emerson, K.-T. Lin, J.N. Gruber, B.S. Donohoe, J.L. Klinger, et al. 2022. "Image Analysis for Rapid Assessment and Quality-Based Sorting of Corn Stover." *Front. Energy Res.* 10: 837698. doi.org/10.3389/fenrg.2022.837698.

Task 3 – Materials Handling

The Materials Handling task develops first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through the processing train to the conversion reactor. Task 3 researchers are developing these tools using advanced computational models describing the transport of bulk solids in hoppers and chutes that have been validated by careful multiscale experimental data. These tools will be available for equipment designers to use to ensure reliable continuous bulk solids handling and transport, and the underlying modeling tools will be shared with the scientific community as open source.

FY 2022 Key Results

Wedge Hopper Design for Woody Biomass

Task 3 researchers performed a parametric study using experimentally validated numerical models for dry woody biomass feedstock in hoppers and identified two hopper properties—wall inclination and wall friction—and one feedstock property—feedstock internal friction—that collectively control flow behavior in the hopper.⁵ They were able to identify parameter combinations that resulted in desirable mass flow behavior

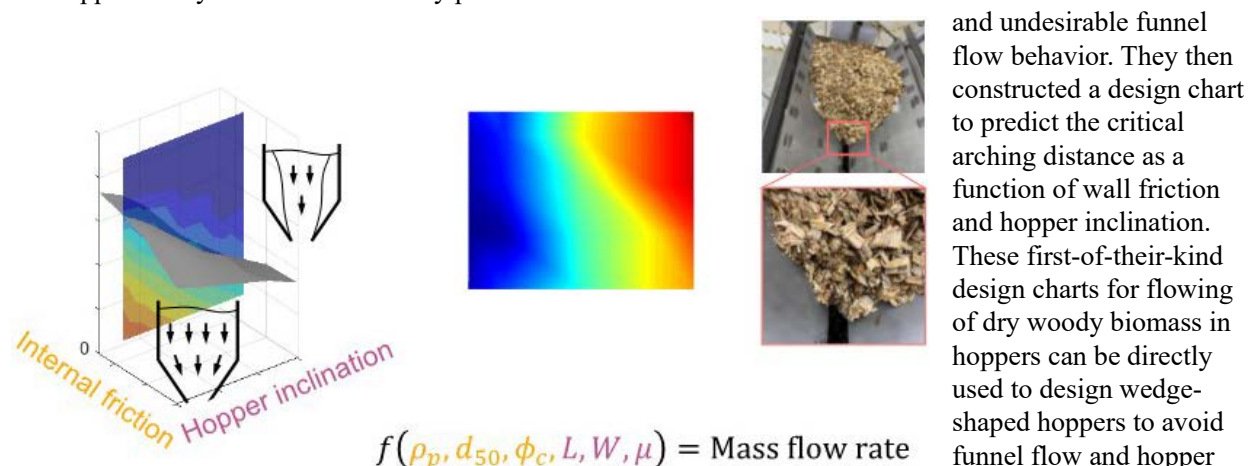


Figure 8. Experimentally validated flow models were used to develop design charts that describe flow behavior in biomass hoppers under different conditions, helping industry stakeholders rapidly design hoppers without needing excessive computational resources.

and undesirable funnel flow behavior. They then constructed a design chart to predict the critical arching distance as a function of wall friction and hopper inclination. These first-of-their-kind design charts for flowing of dry woody biomass in hoppers can be directly used to design wedge-shaped hoppers to avoid funnel flow and hopper arching and to predict throughput for handling dry woody biomass.

Open-Source, Reduced-Order, Discrete Element Method Models

Task 3 researchers completed the open-source release of a discrete element method (DEM) model using reduced-order contact laws to describe the interaction between individual biomass particles.⁶ The reduced-order contact laws reduce the computational requirements for solving the model while still reasonably reproducing experimental results. The model was implemented in the LIGGGHTS-INL open-source DEM particle simulation software and is available to the bioenergy community for use as both a research tool and a design tool.

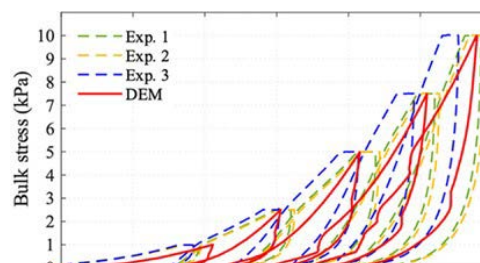


Figure 9. DEM model with reduced-order contact laws can predict stress/strain relationships for woody biomass.

⁵ Y. Lu, W. Jin, N. Saha, J. L. Klinger, Y. Xia, and S. Dai. 2022. "Wedge-Shaped Hopper Design for Milled Woody Biomass Flow." *ACS Sustainable Chemistry & Engineering*. doi.org/10.1021/acssuschemeng.2c05284.

⁶ F. Chen, Y. Xia, J. Klinger, and Q. Chen. 2022. "A set of hysteretic nonlinear contact models for DEM: Theory, formulation, and application for lignocellulosic biomass." *Powder Technology* 397: 117100. doi.org/10.1016/j.powtec.2021.117100. GitHub repository for open-source code is at github.com/idaholab/LIGGGHTS-INL.

Benchmarking Computational Model Performance

Task 3 researchers have been using a combination of computational modeling and robust experimentation to develop design tools to predict the material handling performance of different biomass feedstocks.⁷ In this work the researchers compared both continuum and DEM modeling approaches for predicting granular biomass flow to experimental data. The close agreement of the numerical predictions with the experimental measurements in three classical granular material flow systems demonstrates that both continuum and DEM modeling approaches can capture the critical flow behavior of granular biomass. The continuum mechanics model is preferred for large-scale systems, while the discrete particle model is preferred for discontinuous flow systems at smaller scales. Industry stakeholders can use these findings as guidance for choosing appropriate numerical tools to model biomass material flow.

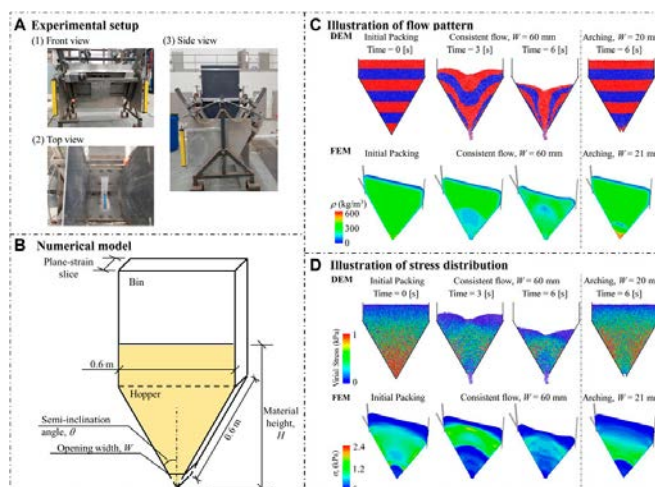


Figure 10. Laboratory experiments coupled with computational modeling can produce useful tools to predict the flow behavior of biomass feedstocks.

Experimental Data on Biomass Flowability

Continuing efforts to generate robust, reproducible experimental data to parameterize and validate computational models, Task 3 executed a series of experiments to measure physical and mechanical attributes of corn stover and pine samples (moisture, particle size distribution, bulk density, compressibility, and elastic recovery) and how these attributes impacted flow behavior (rheological properties, critical arching distance in a wedge hopper, and mass flow rate in a screw feeder).^{8,9} Results for corn stover showed that smaller particle sizes yielded better flowability during screw feeding, and that over the ranges tested, moisture had a less significant impact on flow behavior than particle size.

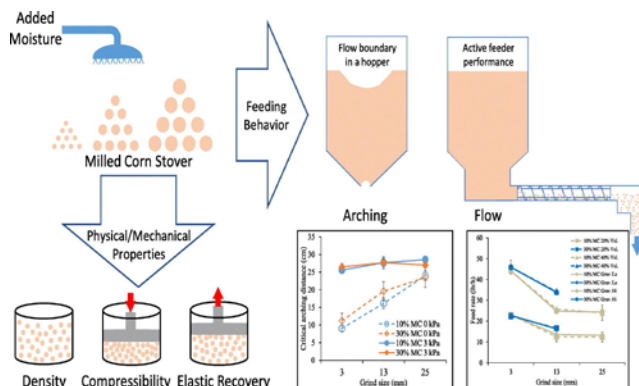


Figure 11 Well-designed experimental campaigns generate robust and reproducible data that are used to understand the intrinsic flow behavior of biomass, and also to parameterize and validate computational models.

FY 2023 Goals

In FY 2023, Task 3 researchers will extend their work on first-principles-based modeling tools to predict the bulk flow of biomass feedstocks to higher-moisture materials, continuing their combined experimental and modeling approach.

⁷ W. Jin, Y. Lu, F. Chen, A. Hamed, N. Saha, J. Klinger, S. Dai, Q. Chen, and Y. Xia. 2022. "On the fidelity of computational models for the flow of milled loblolly pine: A benchmark study on continuum-mechanics models and discrete-particle models." *Frontiers in Energy Research* 10. doi.org/10.3389/fenrg.2022.855848.

⁸ N. Saha, C. Goates, S. Hernandez, W. Jin, T. Westover, and J. Klinger. 2022. "Characterization of particle size and moisture content effects on mechanical and feeding behavior of milled corn (*Zea mays* L.) stover." *Powder Technology*: 117535. doi.org/10.1016/j.powtec.2022.117535.

⁹ R. Navar, J. H. Leal, B. L. Davis, and T. S. Semelsberger. 2022. "Rheological effects of moisture content on the anatomical fractions of loblolly pine (*Pinus taeda*)." *Powder Technology*: 118031. doi.org/10.1016/j.powtec.2022.118031.

Task 4 – Scientific Data Management

The Scientific Data Management task provides a collaborative computational environment for hypothesis development, experimental and modeling workflow management, integration of datasets and metadata, and deliverables sharing between FCIC subtasks, as well as a portal for public access to FCIC results, data, and software. Task 4 provides the necessary infrastructure for FCIC researchers to store and integrate their experimental results according to industry standard guidelines for making data findable, accessible, interoperable, and reusable (FAIR)¹⁰ and to enable easy collaborations among tasks with the FCIC Data Hub, developed in the open-source LabKey environment.

FY 2022 Key Results

QbD Database: The FCIC Data Hub

Task 4 researchers continued their work on the FCIC Data Hub by (1) developing a system for harmonization and database integration of data and metadata specified by Task 8 case studies to support the accrual QbD critical property assignments to biorefinery processes and materials in accordance with FAIR data practices; (2) hosting the initial meeting of the Task 4 Data Stakeholder Advisory Team to optimize the industry relevance of Data Hub resources, formats, and standards; (3) deploying a technology pathway visualization tool on the Data Hub that enables side-by-side comparison of biorefinery block flow diagrams dynamically rendered from data in the technology pathway configurations table; and (4) integrating data and information from two preprocessing-focused and two conversion-focused case studies, journal articles, and technical reports on the Data Hub.

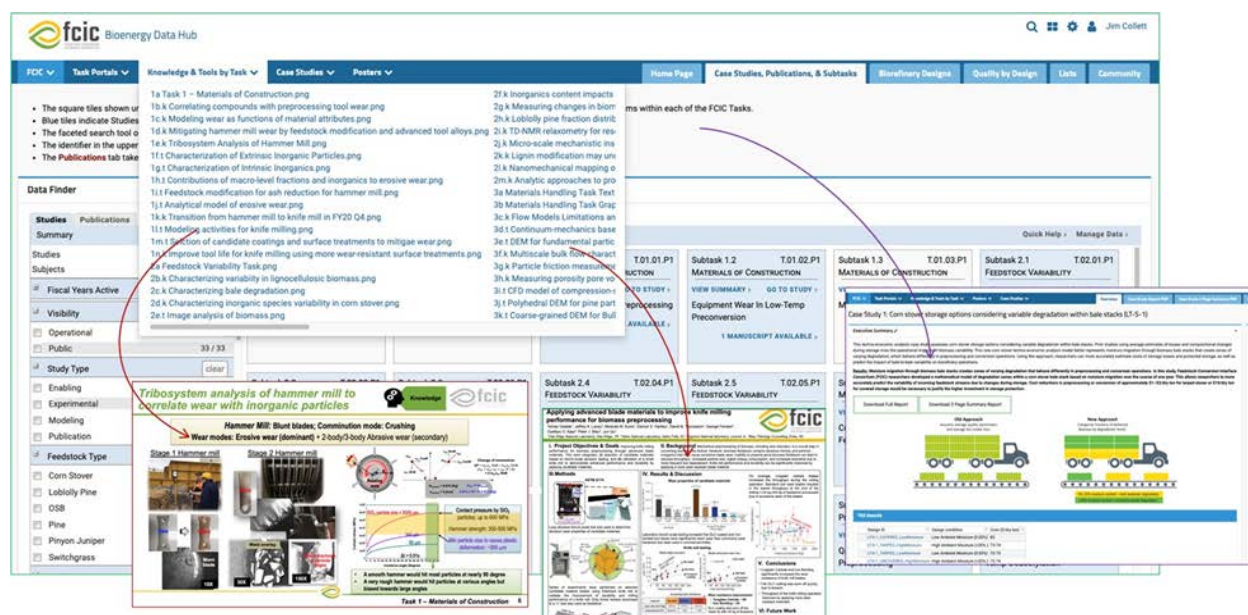


Figure 12. The FCIC Bioenergy Data Hub will allow researchers to quickly and easily share the results of FCIC research to external stakeholders, ensuring FCIC results are FAIR.

FY 2023 Goals

In FY 2023, Task 4 researchers will continue their work to support scientific data management, including deploying the FCIC Data Hub web portal to provide external stakeholders access to the TEA case studies being produced by the FCIC, continuing to update the FCIC Data Hub web portal with curated datasets and publications, and continuing to engage industry stakeholders with recurring workshops.

¹⁰ www.go-fair.org/fair-principles/.

Task 5 – Preprocessing

The Preprocessing task develops science-based design and operation principles informed by TEA/LCA that result in the predictable, reliable, and scalable performance of preprocessing unit operations. The task is providing knowledge and tools to industry stakeholders through fundamental studies of comminution and deacetylation that produce validated mechanistic models that predict how feedstock material attributes and process parameters of milling and deacetylation produce feedstocks with quality attributes required by downstream conversion.

FY 2022 Key Results

Microstructural and Mechanical Model

Continuing their work to develop robust comminution models for biomass resources, FCIC Task 5 researchers demonstrated the agreement and consistency of microscale and macroscale models and laboratory experiments.¹¹ In this work, the team investigated two different approaches for downscaling parameters from macroscale experiments for use in microscale DEM models and showed that microscale DEM models can predict the Young's modulus in general agreement with experimental measurements. Example code from this work has been shared in the open-source LIGGGHTS-INL repository at github.com/idaholab/LIGGGHTS-INL.

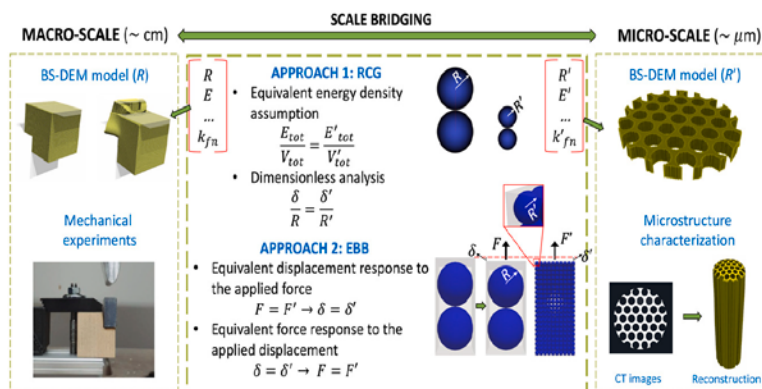


Figure 13. By using appropriate downscaling methods, it is possible to successfully parametrize microscale models using data from macroscale mechanical experiments.

Molecular Modeling of Biopolymer Assembly Strength

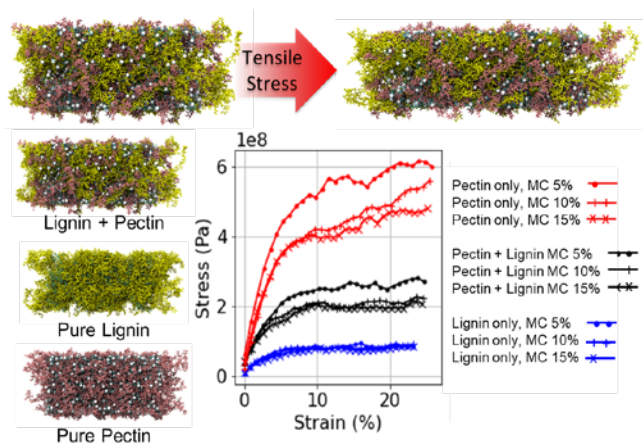


Figure 14. Molecular dynamics modeling reveals how variations in moisture content and composition show variable composition and lead to dramatic changes in variable mechanical properties of biopolymer assemblies.

The ability to predict macroscale physical and mechanical behavior of biomass from ubiquitous characterization like compositional analysis requires fundamental knowledge of how molecular-scale forces propagate through hierarchical biomass structures. Task researchers used molecular modeling to study the stress/strain relationships of varying moisture, lignin, and pectin compositions typical of the middle lamella tissue type. This work showed that pure pectin assemblies are much stiffer than pure lignin assemblies, and that lignin acts as a plasticizer in the middle lamella. These molecular modeling studies identify the chemical origins of biomass feedstock physical and mechanical properties and help predict preprocessing behavior based on biopolymer composition.

¹¹ Q. Sun, Q. Chen, Y. Xia, F. Chen, J. Klinger, L. Ding, and V. Thompson. 2022. "Reverse scaling of a bonded-sphere DEM model: Formulation and application to lignocellulosic biomass microstructures." *Powder Technology* 407: 117797. [dx.doi.org/10.1016/j.powtec.2022.117797](https://doi.org/10.1016/j.powtec.2022.117797).

Comminution Modeling

Robust, reproducible experimental data on the physical, chemical, or mechanical properties of biomass resources address a key source of uncertainty for the design of biomass handling equipment and processes. FCIC Task 5 researchers developed a novel three-point cyclic bending-recovery experiment to highlight elastic deformation followed by incremental structural damage, describing the elastoplastic flexural behavior of corn stalks.¹² These data provide substantial insight to the physical and mechanical behavior of corn stover under stress and how the behavior varies within a single corn stalk and at different scales. The data are also invaluable for the parameterization and validation of computational models (e.g., DEM) that can predict the flow behavior of biomass materials like corn stover and inform structural deformation models of the corn stover itself.

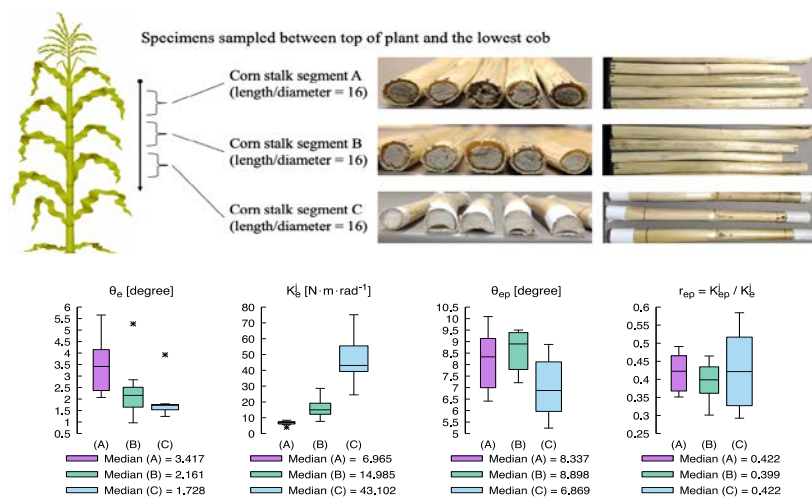


Figure 15. Experimental biomechanical property data of corn stover are critical for the parameterization and validation of comminution models.

MRF Residue Characterization

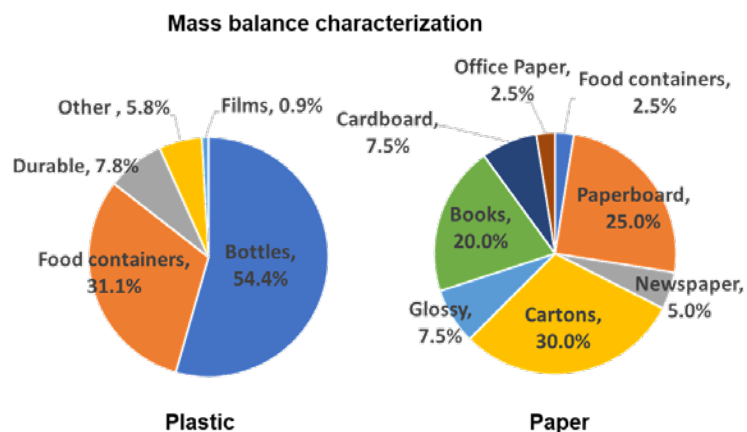


Figure 16. Fractionated post-MRF residues have different compositions, leading to different chemical, physical, and mechanical properties.

Task 5 researchers took the lead for the FCIC in acquiring landfill-bound residue from a single-stream MRF. The bales of material were deconstructed at the Idaho National Laboratory Biomass Feedstock National User Facility, air-classified into plastics-rich and paper-rich fractions, reduced in size, and then shared with other FCIC researchers. The plastics-rich and paper-rich streams had very different constituents, resulting in very different chemical and physical attributes. Successful utilization of cost-advantaged feedstocks like MRF residues depends on a thorough understanding of their properties.

FY 2023 Goals

In FY 2023, Task 5 researchers will continue their combined experimental and multiscale modeling work to understand the physical and mechanical behavior of biomass resources and representative MRF residues during preprocessing, and to develop tools for rapid characterization of biomass composition and conversion performance.

¹² Y. Xia, J. Klinger, T. Bhattacharjee, and V. Thompson. 2022. "The elastoplastic flexural behavior of corn stalks." *Biosystems Engineering* 216: 218–228. doi.org/10.1016/j.biosystemseng.2022.02.016.

Task 6 – High-Temperature Conversion

The High-Temperature Conversion task develops the science-based understanding required to accurately predict the effects of variable feedstock attributes and process parameters on gasification and fast pyrolysis product quality attributes. Task 6 researchers are developing validated, multiscale experimental and computational frameworks to allow thermochemical conversion biorefineries to maximize productivity and product quality with variable incoming feedstock attributes.

FY 2022 Key Results

Biomass Degradation in Auger Feeders

Feeding biomass into high-temperature conversion reactors can be complicated if thermally induced degradation of the biomass occurs in the feed system rather than in the conversion reactor itself. Thermal degradation can result in material deposition in the feeding system, causing feeding interruptions. In this work, Task 6 researchers investigated the effect of pine residue variability on material deposition on an auger screw feeder connected to a laboratory-scale fluidized-bed pyrolysis reactor.¹³ They showed that if the pine residue consisted of cleaner material (e.g., more white wood, less bark) there was less material deposition on the screw feeder. Chemical analysis of the volatile organic compounds released from the biomass samples showed substantial differences in composition depending on the devolatilization temperature. Computer simulations of the temperature profile of the auger system confirmed that substantial temperature gradients exist across the length of the feed auger, and that water cooling is far superior to air cooling to minimize biomass thermal degradation in the feed system.

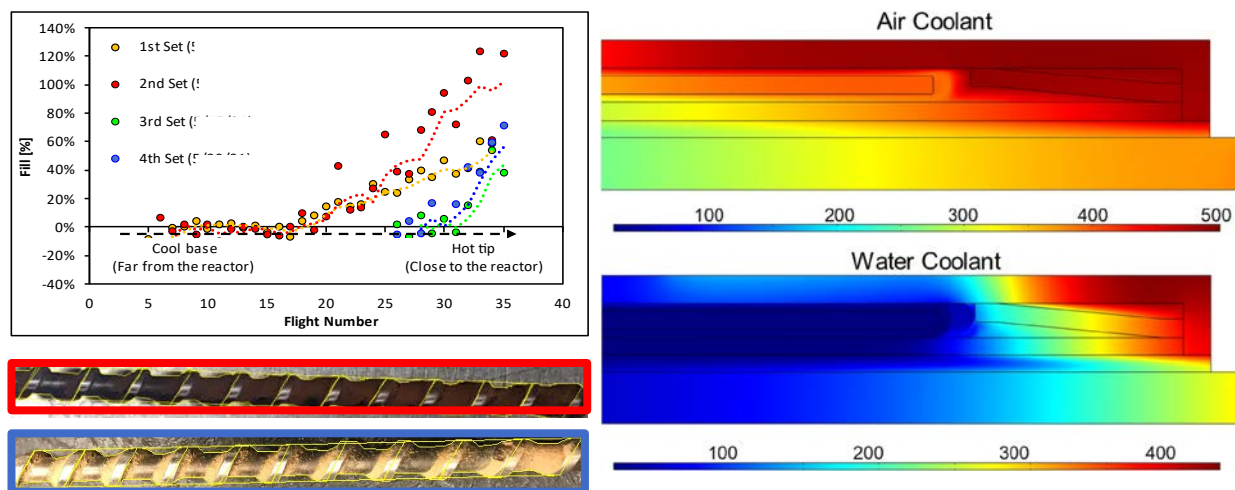


Figure 17. Experimental and modeling investigations of a laboratory-scale auger feeder demonstrated large differences in thermal degradation of biomass in the feed system depending on the pine residue composition and the operating conditions, and clearly showed the advantages of water cooling versus air cooling.

Adding Gasification as a Pathway

In FY22, Task 6 researchers expanded their multiscale modeling and experimental approach to include both fast pyrolysis and gasification, with both pathways eventually leading to sustainable aviation fuel (SAF). The fast pyrolysis pathway is likely more amenable to biomass feedstocks, while the gasification pathway will likely be the preferred pathway for more heterogeneous materials like MSW.

¹³ N. Saha, J. Klinger, S. Rowland, T. Dunning, D. Carpenter, Z. Mills, and J. Parks. 2022. "Influence of feedstock variability on thermal decomposition of forest residue in a screw feeder for high temperature conversion." *Fuel Processing Technology* 245: 107725. doi.org/10.1016/j.fuproc.2023.107725.

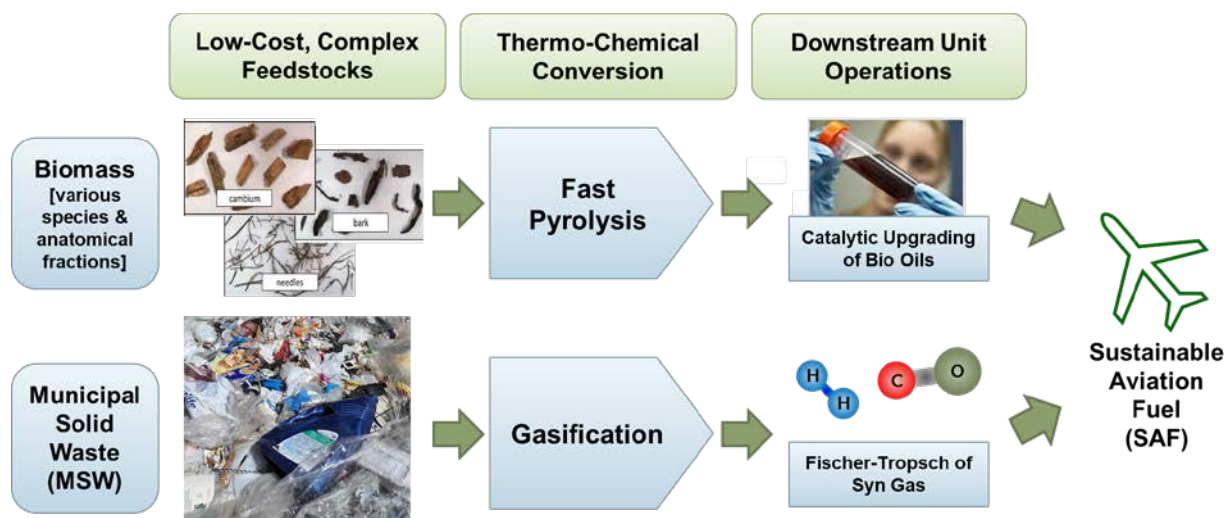


Figure 18. Validated, multiscale experimental and computational frameworks for both fast pyrolysis and gasification will support SAF production by providing tools for biorefineries to predict critical product quality attributes from variable feedstock CMAs.

Thermal Stability of Pyrolysis Bio-Oils

Task 6 researchers investigated the thermal stability of CFP bio-oils, which need hydrotreating to remove unwanted oxygen from the oils. They showed that higher temperatures and longer residence times during bio-oil heat treatment increased the viscosity of the oils dramatically, and modestly increased the average molecular weight, indicating some oligomerization was occurring. Understanding the stability of CFP bio-oils is critical to designing a complete conversion system leading from biomass resources through liquid intermediates to SAF.

FY 2023 Goals

In FY 2023, Task 6 researchers will continue their combined multiscale modeling and experimental approach to develop a robust, science-based understanding of the effects of feedstock variability on both fast pyrolysis and gasification conversion pathways. They will bring additional gasification and pyrolysis experimental tools online to support the parametrization and validation of their multiscale models, and continue external collaborations with industry and academic partners.

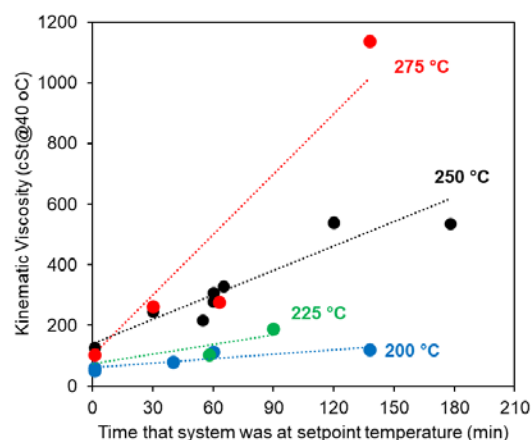


Figure 19. Thermal stability testing of CFP bio-oils shows oil viscosity rose dramatically with increasing time and temperature, which can cause plugging in the hydrotreater.

Task 7 – Low-Temperature Conversion

The Low-Temperature Conversion task determines the effects of biomass feedstock variability on unit operation required for low-temperature conversion processes (utilizing both sugar and lignin pathways) and develops tools to mitigate the risks posed by this variability. The first-principles-based knowledge and tools generated by this team will help mitigate the risks posed by feedstock variability to enable the prediction of bioconversion performance on future low-temperature processes.

FY 2022 Key Results

Drought Stress Does Not Affect Corn Stover Pretreatment Performance

While drought is known to adversely affect overall corn (and therefore corn stover) harvest yields, there is little known about the relative performance of drought corn stover during biochemical conversion to cellulosic sugars. Task 7 researchers compared drought-stressed and control corn stover deconstruction performance in three different pathways and showed that drought-stressed corn stover (in bulk or as fractionated into air classification) performs similarly to non-drought-stressed corn stover with respect to biomass digestibility; variation between the anatomical fractions is similar in both. Thus, drought, which has been hypothesized to be a critical source of feedstock variability, appears to have a relatively minor impact on low-temperature conversion, removing a significant source of uncertainty for biorefineries.

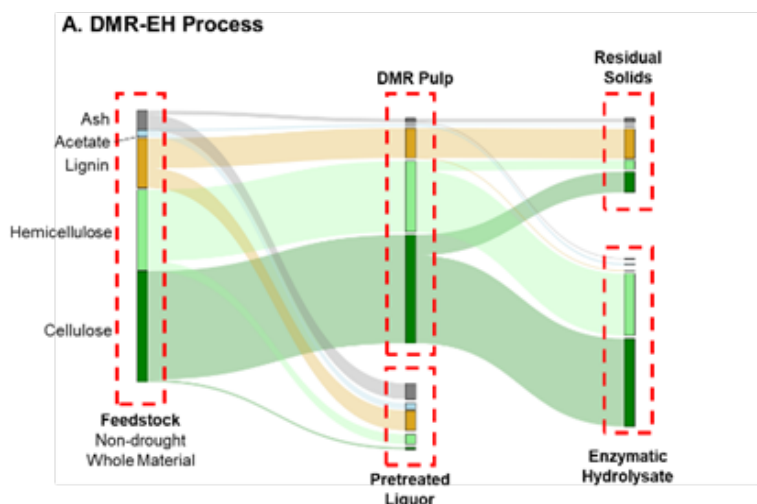


Figure 20. Sankey diagram showing carbon flows for one of the three deconstruction pathways examined—DMR. Drought did not affect the performance of corn stover samples in any deconstruction pathway.

Inhibitory Compounds from Deacetylation Are Easily Mitigated

Public data regarding the impact of feedstock variability on the performance of organisms in fermentation processes using sugar streams derived from DMR-pretreated biomass are unknown/underrepresented. Task 7 researchers systematically evaluated 25 different material attributes in cellulosic sugar streams produced from the enzymatic hydrolysis of DMR-treated corn stover to identify those that are inhibitory to *Clostridium tyrobutyricum*. The top five CMAs were sodium, ferulate, coumarate, ammonium sulfate, and lactic acid. However, the inhibitory effects of all identified inhibitory compounds can be effectively mitigated by washing the solids after DMR but before the enzymatic hydrolysis. Thus, the inhibitory compounds typical of DMR do not appear to represent a significant risk to the scale-up of this deconstruction pathway.

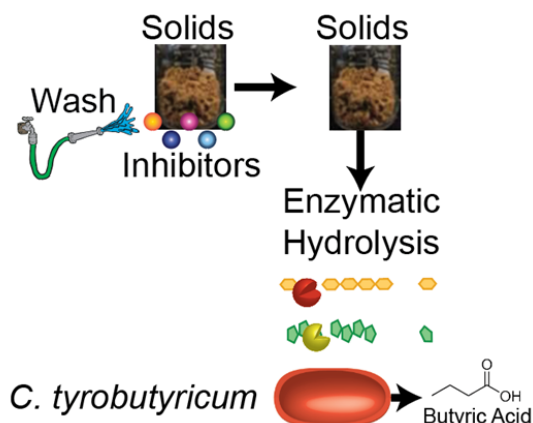


Figure 21. Washing solids from the DMR process removes inhibitory compounds and results in sugar streams readily fermentable by *C. tyrobutyricum*.

Top CMAs for Muconate Production by Pseudomonas putida (P. putida) in Deacetylation Black Liquors Become Inhibitory Only in Concentrated Lignin Streams

Task 7 researchers determined the concentrations that inhibit growth in *P. putida* rates by 25% and 75% (EC25 or EC75) for the top three CMAs in deacetylation black liquor: sodium sulfate, sodium chloride, and sodium nitrate. However, these sodium salts become inhibitory only at concentration values substantially above those typical of deacetylation. In addition, combinations of the top five CMAs did not produce any synergistic effects on *P. putida* performance, only additive effects. These results increase our understanding of the DMR process, inform the design of other DMR process configurations, and provide useful approaches to optimize the biocatalyst to tolerate higher salt concentrations.

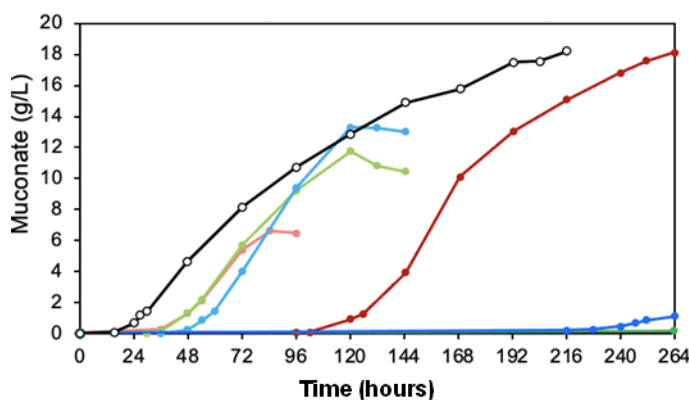


Figure 22. Muconate production by *C. tyrobutyricum* is inhibited by the sodium salts of sulfate, chloride, and nitrate present in deacetylation black liquor only when the liquor is concentrated.

FY 2023 Goals

In FY 2023, Task 7 researchers will continue their interdisciplinary approach to continue development and validation of the capstone output of Task 7—a validated artificial intelligence tool able to predict the performance of new organisms on variable sugar and lignin streams. This tool will enable industry stakeholders to estimate the performance of new strains rapidly and help to define appropriate upstream operations that allow sugar and lignin stream composition to be constrained for optimal microbial conversion performance.

Task 8 – Crosscutting Analyses

The Crosscutting Analyses task quantifies and communicates industrially relevant cost and environmental impacts for the results of FCIC research. The interdisciplinary Crosscutting Analyses task leverages well-documented and robust BETO-supported TEA and LCA modeling resources¹⁴ to quantify how feedstock variability affects underlying economics and sustainability metrics through the entire value chain, from feedstock production through preprocessing and conversion. The results of these analyses are being presented in the form of case studies—TEA or LCA focused on a specific process or group of processes within the bioenergy value chain. The results of these case studies allow industry stakeholders to quickly understand the economic sustainability implications of feedstock variability for specific unit operations and at a systems level, as well as to help focus ongoing FCIC research efforts to address areas where feedstock variability is most impactful.

FY 2022 Key Results

Wear-Resistant Knife Blades Can Save Money

The ash component in biomass feedstocks leads to wear and other forms of surface damage, which causes excessive downtime due to frequent mill maintenance and blade replacement. This work examined the value of using more expensive wear-resistant knife blades in knife-milling unit operations and showed that using more expensive blades can reduce the overall operational cost of a knife mill, despite the higher cost, by increasing the interval between knife blade replacement, resulting in less downtime. The exact savings depended on the wear-resistant material used.

Air Classification for Optimized Conversion Performance

Sequential air classification to enrich corn stover material into anatomical fractions would facilitate running sequential downstream conversion campaigns with conditions optimized for each enriched anatomical fraction, since previous FCIC research showed the conversion performance of different corn stover anatomical fractions were very different. This work suggested that the potential gains in conversion performance will more than offset the costs for air classification, although thoughtful design of the preprocessing and conversion systems will be necessary.

Review of Gasification Models

Various BETO-funded gasification models have been developed over the years that could be used to support future TEA efforts in the FCIC. The key limitation in using these models going forward is a lack of robust experimental data to update the feedstock/product correlations used in these models, since the original correlations were derived from experiments with woody feedstocks rather than MSW materials, a key interest of the FCIC.

Drought-Stressed Corn Stover Conversion Performance

Two corn stover harvests from the same location during two different years—one with normal precipitation and one with substantially less precipitation than normal—were tested using two different conversion preprocessing pathways: DMR followed by enzymatic hydrolysis and dilute acid pretreatment followed by enzymatic hydrolysis. The TEA screening assessment found relatively small differences in performance between the normal and drought-stressed corn stover for both DMR and dilute acid pretreatment, with generally more favorable economics for the DMR process compared to the dilute acid process.

LCA Impacts of MSW Management

A preliminary review of the sustainability opportunities related to using MSW components to produce fuels showed significant emissions improvements from diverting these MSW components from the landfill for use

¹⁴ bioenergymodels.nrel.gov/models.

in biofuels production, including the displacement of petroleum-derived fuel plus and the avoidance of landfill-related decomposition and greenhouse gas emissions from these MSW components.

Pine Tree Thinnings and Pine Residue Supply Costs

The total delivered cost of biomass from pine thinning operations (required as part of plantation operations) was more expensive than supplying only harvest residues (the tops and limbs removed as mature trees are processed immediately after timber harvest). Combined scenarios, where some tree thinnings and some harvest residues are used in the biomass supply chain, had supply costs between the two options.

Air Classification Has Minimal LCA Impacts

The LCA impact of air classification in feedstock preprocessing on the life cycle greenhouse gas emissions of fuels produced via CFP were minimal because of the modest energy use compared to the main preprocessing unit operations of biomass drying and comminution, and depended primarily on the extent of the air classification.

FY 2023 Goals

In FY 2023, Task 8 researchers will continue their work to quantify and communicate the impacts of FCIC research through well-documented case studies covering both the low- and high-temperature conversion pathways. Approximately 10 additional case studies are planned for FY 2023, including the integration of existing single-unit operation case studies to examine systemwide effects.

Task 8 researchers will also be working with FCIC and BETO leadership to share the results of these case studies with external stakeholders using a variety of communication tools, including the FCIC website (www.energy.gov/fcic), conference presentations, and trade journals.





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