U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Annual Review of Research
FY 2021

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Disclaimer

List of Acronyms

BETO	Bioenergy Technologies Office
DMR	deacetylation and mechanical refining
FCIC	Feedstock-Conversion Interface Consortium
FY	fiscal year
LCA	life cycle analysis
MSW	municipal solid waste
QbD	quality by design
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 (BETO) 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.

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 harvest and storage process area; 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 second annual report from the FCIC and presents an overview of the research accomplishments of FCIC members in fiscal year (FY) 2021, 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 2022 work that will build on the FY 2021 accomplishments.

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.

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 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.

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.

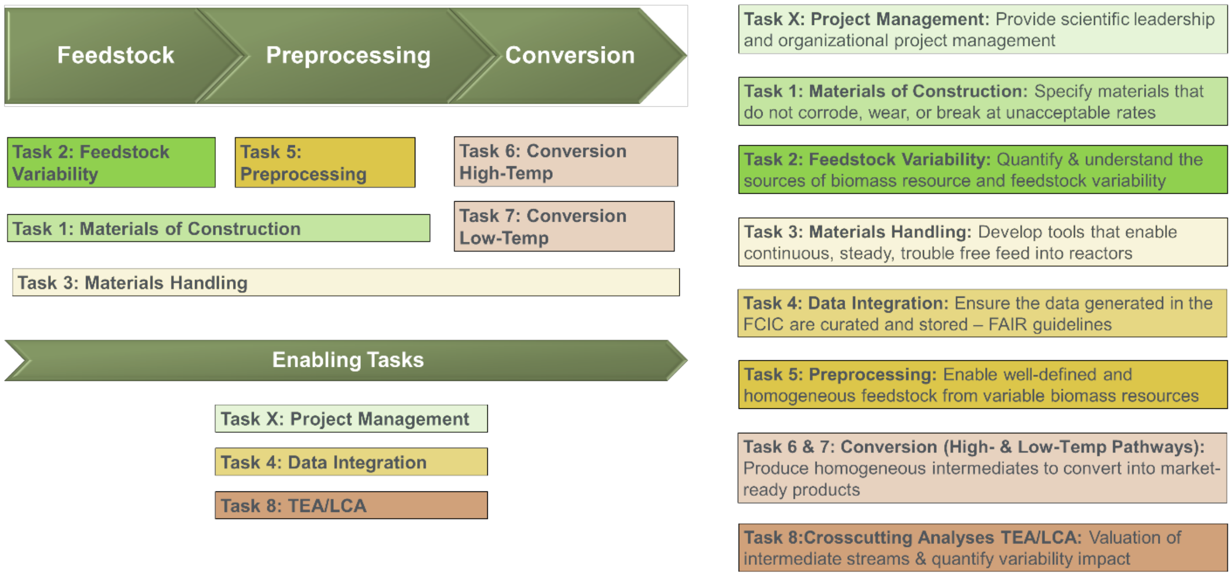

Figure 1. FCIC tasks span feedstock, preprocessing, and conversion areas, with enabling tasks spanning the project.

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), 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.

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[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. https://www.fda.gov/about-fda/center-drug-evaluation-and-research-cder/pharmaceutical-quality-21st-century-risk-based-approach-progress-report.

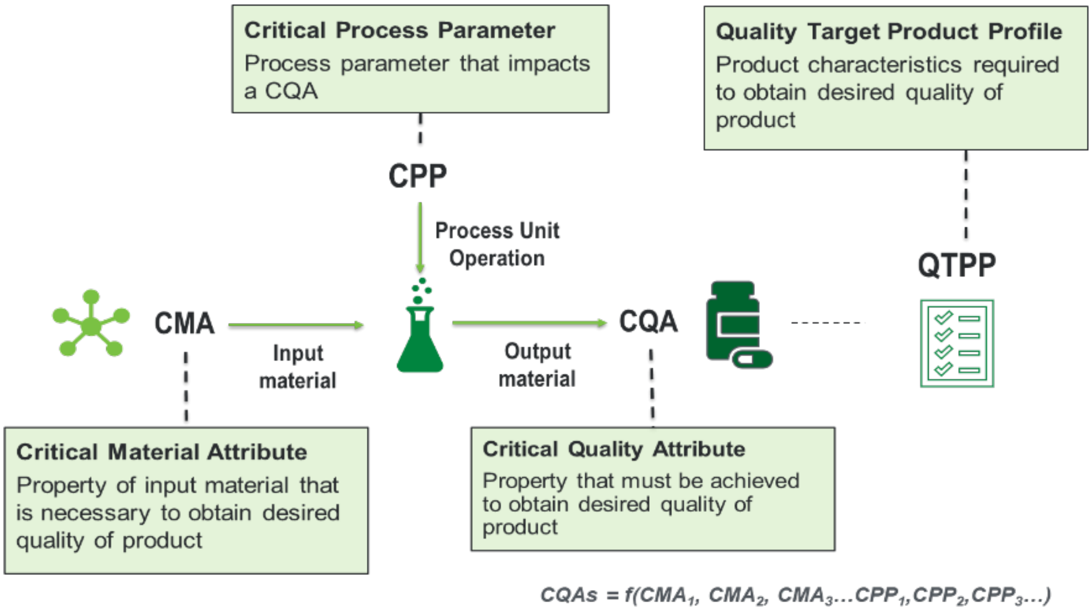


Figure 2. QbD parameter names and descriptions

Task Accomplishments

This report presents a high-level overview of the accomplishments of the FCIC in fiscal year (FY) 2021, 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 2022 work that will build on the FY 2021 accomplishments. A full list of publications is available on the FCIC website: https://www.energy.gov/eere/bioenergy/fcic-publications.

Task 1 – Materials of Construction

The objective of the Materials of Construction task is to use 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.

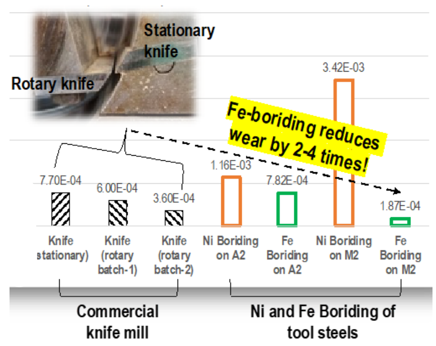


Figure 4. Surface treatments decrease wear of knife-mill blades by 2–4 times.

FY 2021 Key Results

Understanding Mechanisms of Wear

Task 1 researchers demonstrated that different comminution equipment exhibit fundamentally different mechanisms of wear. For example, wear in hammermills is largely due to erosion,[3] wear in rotary shear mills is largely due to abrasion,[4] and wear in knife mills involves both modes. Understanding these different mechanisms is critical for developing cost-effective approaches to mitigate the impact of wear on biomass processing equipment.

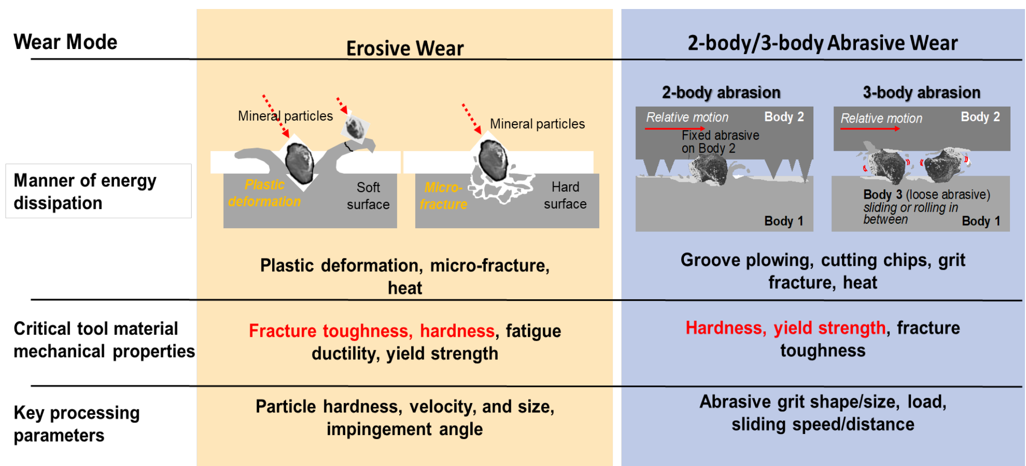


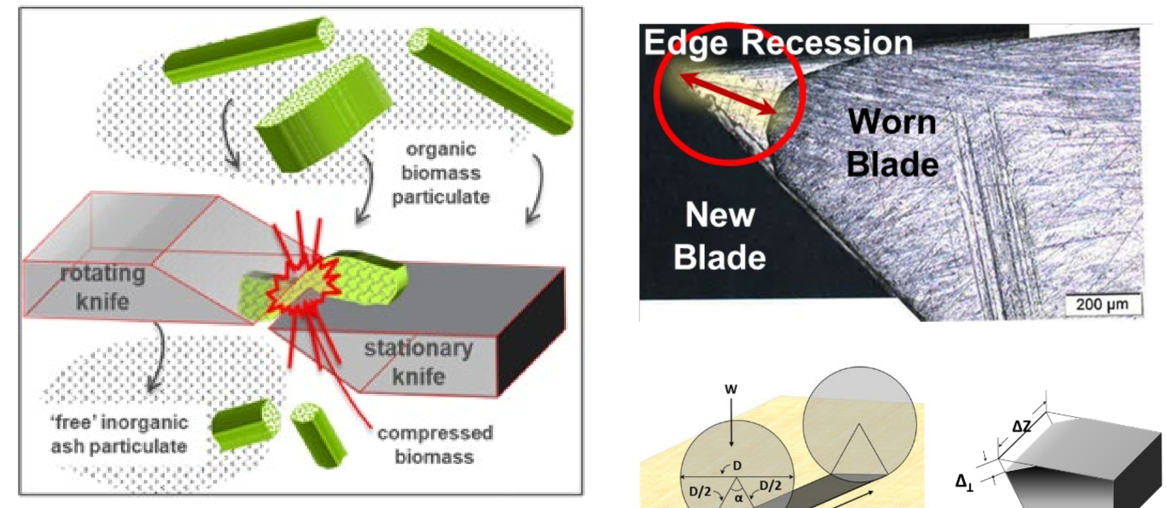
Figure 3. Understanding the specific mechanisms causing wear in biomass processing equipment is critically important to design cost-effective mitigation approaches.

Low-Cost Surface Treatments Improve Wear Resistance

It may be possible to use wear-resistant surface treatments and surface treatments to mitigate blade wear during biomass processing. Task 1 researchers examined several potential coatings in laboratory experiments and performed larger-scale experiments with two coatings. Both iron boride (FeB) and "diamond-like carbon" (DLC) coatings showed significant promise as low-cost wear mitigation approaches. The experimental work included laboratory wear testing, detailed chemical and surface characterization, and extended experiments with biomass samples to understand how these coatings affect the fundamental wear mechanisms that are occurring and to predict how these coatings will perform under industrially relevant conditions.

[3] K. Lee, D. Lanning, L. Lin, E. Cakmak, J.R. Keiser, and Jun Qu. 2021. "Wear Mechanism Analysis of a New Rotary Shear Biomass Comminution System." *ACS Sustainable Chemistry & Engineering* 9 (35): 11652–11660. https://doi.org/10.1021/acssuschemeng.1c02542.

[4] S. Roy, K. Lee, J.A. Lacey, V.S. Thompson, J.R. Keiser, and J. Qu. 2020. "Material Characterization-Based Wear Mechanism Investigation for Biomass Hammer Mills." *ACS Sustainable Chemistry & Engineering* 8 (9): 3541–3546. https://doi.org/10.1021/acssuschemeng.9b06450.



$$\Delta_{\perp} = \left(\frac{1}{2}\right)\left(\frac{D_p}{2}\right)^2 * (\alpha - sin\alpha) * \mathcal{X} * \frac{\pi}{4} N_{chip} D_{chip}^2$$

Figure 5. The ABRADE spreadsheet model uses knife-mill process parameters, critical material attributes of the inorganic mineral species in feedstock, and the physical and mechanical attributes of the knife blades to predict the rate of abrasive wear in knife-mill blades.

Open-Source Model for Knife-Mill Blade Wear

A key step away from empirical approaches to manage material wear is the use of first-principles-based mathematical models to predict how specific materials will behave when subjected to wear-inducing materials. Task 1 researchers developed an analytical model to predict the edge recession in knife-mill blades based on the chemical, physical, and mechanic properties of the knife-mill blades; the inorganic species present in the biomass; and the operating parameters of the knife mill. This work was documented in a series of technical reports,[5,6,7,8] and the resulting model is now available as an open-source tool for industry stakeholders at https://www.anl.gov/amd/abrade-model.

FY 2022 Goals

In FY 2022, Task 1 researchers will continue their work to understand the effects of biomass feedstock and process variability on wear in knife mills used in preprocessing. This work will include completing a case study (in collaboration with Task 8 – Crosscutting Analyses) on the economics of knife mill wear mitigation, comparing increased capital costs caused by materials substitution or surface treatments with decreased operating costs due to decreased maintenance costs and increased tool life. They will also begin work in collaboration with industry stakeholders to extend their work with biomass feedstocks into municipal solid waste (MSW) materials.

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[5] George Fenske and Oyelayo Ajayi. 2020. *An Analytical Model of Erosive Wear of BioMass Comminution Components*. Lemont, IL: Argonne National Laboratory. ANL/AMD-20/1. https://www.osti.gov/biblio/1734866-analytical-model-erosive-wear-biomass-comminution-components.

[6] George Fenske and Oyelayo Ajayi. 2020. *Application of an Erosion Wear Model to Predict Wear of Hammer Milling Components*. Lemont, IL: Argonne National Laboratory. ANL/AMD-20/2. https://www.osti.gov/biblio/1763729-application-erosion-wear-model-predict-wear-hammer-milling-components.

[7] George Fenske and Oyelayo Ajayi. 2020. *Identification of Critical Process Parameters for Knife Milling and Alternative Communication Strategies*. Lemont, IL: Argonne National Laboratory. ANL/AMD-20/3. https://www.osti.gov/biblio/1767136-identification-critical-process-parameters-knife-milling-alternative-communication-strategies.

[8] George Fenske and Oyelayo Ajayi. 2021. *An Abrasive Wear Model of Knife Milling to Predict the Impact of Material Properties and Milling Parameters on Knife Edge Recession*. Lemont, IL: Argonne National Laboratory. ANL/AMD-21/3. https://doi.org/10.2172/1818971.

Task 2 – Feedstock Variability

The objective of the Feedstock Variability task is 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, genetics, harvest conditions, degradation during storage) will enable the identification and quantification of material attribute variability that propagates across the value chain. Task 2 researchers work closely with other FCIC researchers to share their fundamental learnings on the magnitude and potential impacts of feedstock variability across the bioenergy value chain.

FY 2021 Key Results

Variability of Inorganic Composition in Woody Biomass

Task 2 researchers provided a critical review of sources and variability of inorganic species in woody biomass, providing insight on how specific inorganic species, their variability, and transport behavior impact downstream conversion of woody biomass.[9] This work comprehensively reviewed inorganic species concentration in woody biomass based on anatomical fractions and their sources of variability and discussed the advantages and disadvantages of characterization techniques for quantifying inorganic elements in biomass, as well as considerations on the impacts of inorganic species on preprocessing and high-temperature conversion processes such as pyrolysis. Finally, it discussed strategies to mitigate the negative impacts of inorganic species present in woody materials. This review provides insights on critical feedstock quality specification and management strategies required for preprocessing and high-temperature conversion.

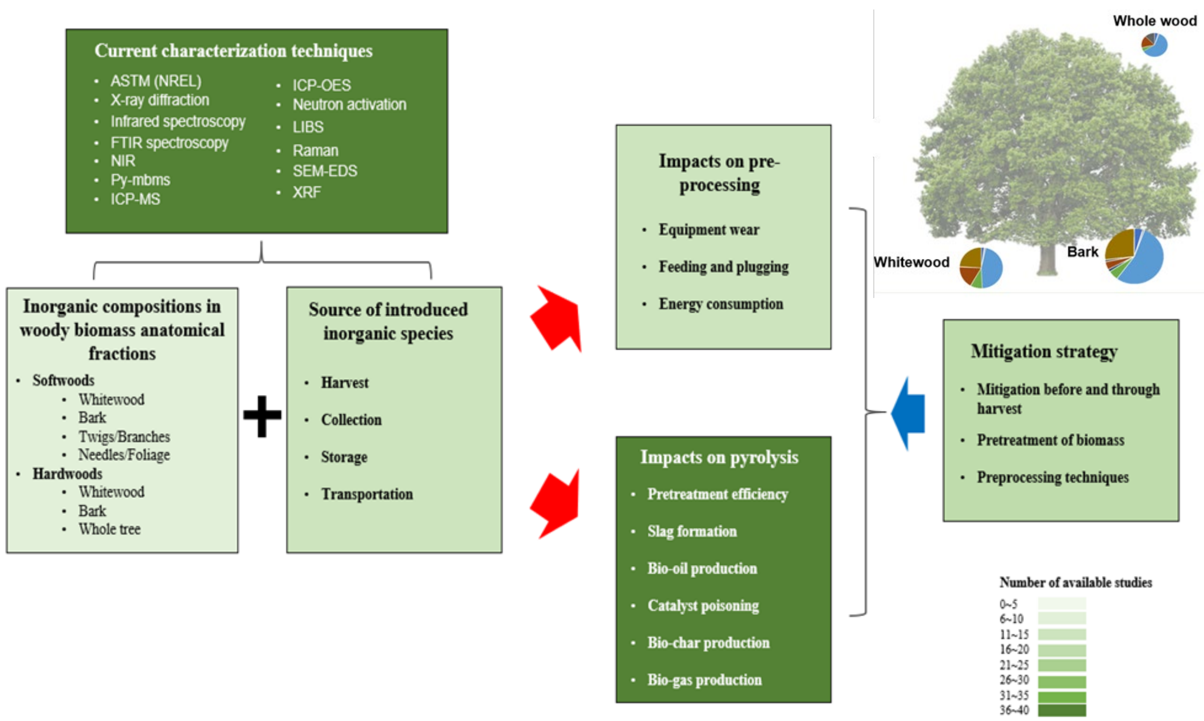

Figure 6. Measuring the intrinsic variability of inorganic species in woody biomass is critical to designing robust processes to mitigate the impact of this variability on preprocessing and conversion pathways.

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[9] L. Ding, Y. Lin, K.-T. Lin, K. Sale, B. Donohoe, A. Ray, C. Li. 2022. "Variability, Transport, and Impacts of Inorganic Species in Woody Biomass—A Review." *Renewable & Sustainable Energy Reviews*, under review.

TD-NMR Relaxometry Reveals Water Distribution in Anatomical Fractions

While the moisture content of biomass is a known critical material attribute for multple unit operations in the bioenergy value chain, the influence of water on biomass properties is complex. It cannot be captured and understood by measuring only the bulk moisture content of a biomass sample. Task 2 researchers investigated the distribution of water within biomass tissues and how it interacted with biomass microstructure to influence physical and chemical changes during storage and preprocessing

Task 2 researchers applied multiple analytical techniques[10] including time-domain nuclear magnetic resonance (TD-NMR) spectroscopy and scanning electron microscopy (SEM) to understand the influence of local environments in porous materials and elucidate water interactions in corn stover and pine residue feedstocks, including samples that had undergone biological degradation during storage. This work provided insights into the microstructure, wettability, and chemical environments within biomass materials that impact water diffusion rates, enzyme access, and overall recalcitrance of lignocellulosic biomass, demonstrating the practical value of advanced characterization tools to inform biomass harvest and storage best practices.

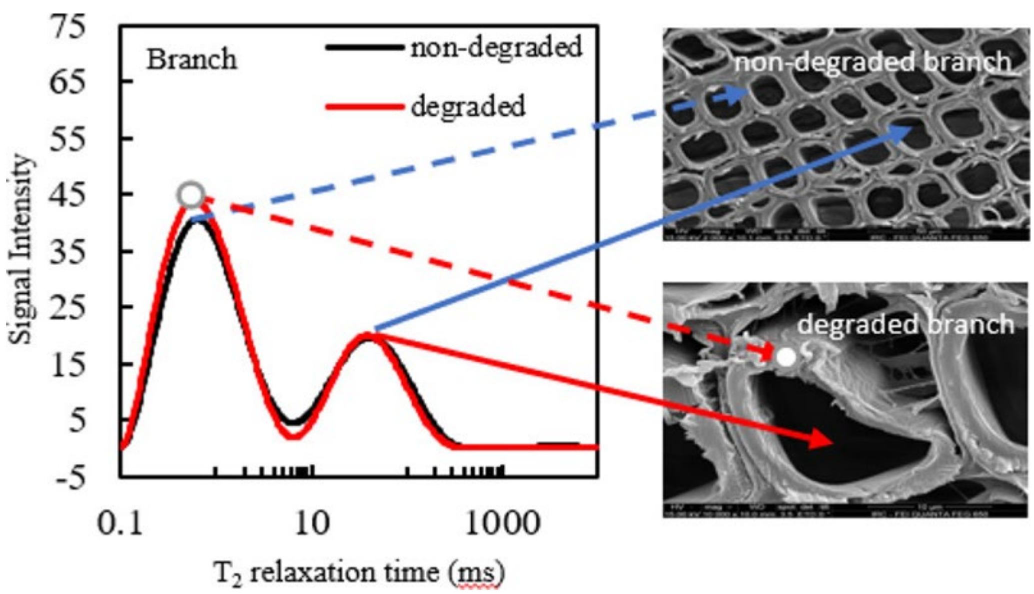

Figure 7. Time-domain nuclear magnetic resonance (TD-NMR) spectroscopy shows the changes in water pool distributions (as measured by T_2 relaxation times) in pine bark samples.

FY 2022 Goals

In FY 2022, 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 translating their primary scientific findings into actionable heuristics and guidelines that stakeholders can use to minimize the impact of feedstock variability across the bioenergy value chain. Finally, they will be applying their characterization tools to representative MSW samples.

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[10] Ling Ding, Josephine N. Gruber, Allison E. Ray, Bryon S. Donohoe, and Chenlin Li. 2021. "Distribution of Bound and Free Water in Anatomical Fractions of Pine Residues and Corn Stover as a Function of Biological Degradation." *ACS Sustainable Chemistry & Engineering* 9 (47): 15884–15896. https://doi.org/10.1021/acssuschemeng.1c05606.

Task 3 – Materials Handling

The objective of the Materials Handling task is to develop 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 2021 Key Results

Developed and Demonstrated Multiscale Bulk Flow Characterization

FCIC researchers continued to develop and implement multiscale characterization methods and paired them with flow validation data to correlate material attributes with bulk flow performance.[11] Current test methods do not always provide data that can be used to directly predict flow performance of biomass in pilot test equipment developed for powders and soils. For example, particle-particle and particle-surface friction was found to depend on particle size and orientation as well as wall material properties. These experimental capabilities allow the capture of complex interactions of biomass anisotropic compressibility, bulk creep, surface properties and morphology, and biomass heterogeneity and variability. These improved experimental capabilities allow better data,[12] resulting in an improved understanding of how biomass material properties impact flow performance and better-informed modeling.[13]

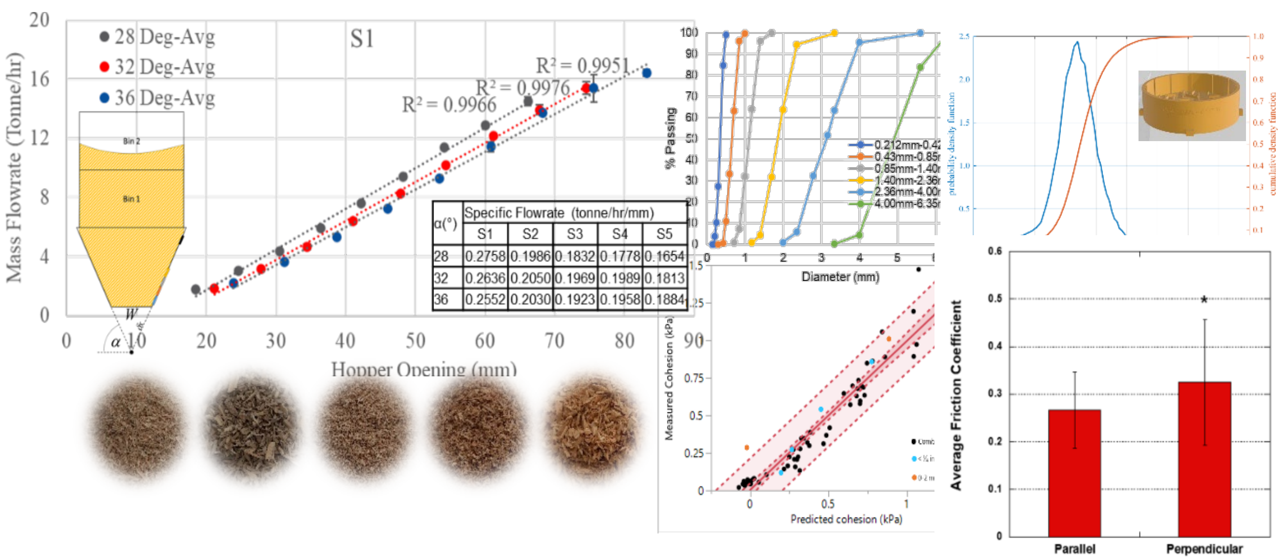

Figure 8. Multiscale bulk flow characterization tools developed by FCIC researchers. These tools are critical to understand the flow behavior of biomass feedstocks and to parameterize and validate advanced computational flow models.

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[11] Ziwei Cheng, Juan H. Leal, Carrie E. Hartford, John W. Carson, Bryon S. Donohoe, David A. Craig, Yidong Xia, Richard C. Daniel, Oyelayo O. Ajayi, and Troy A. Semelsberger. 2021. "Flow behavior characterization of biomass Feedstocks." *Powder Technology* 387: 156–180. https://doi.org/10.1016/j.powtec.2021.04.004.

[12] Yimin Lu, Wencheng Jin, Jordan Klinger, and Sheng Dai. 2021. "Flow and Arching of Biomass Particles in Wedge-Shaped Hoppers." *ACS Sustainable Chemistry & Engineering* 9 (45): 15303–15314. https://doi.org/10.1021/acssuschemeng.1c05628.

[13] Yimin Lu, Wencheng Jin, Jordan Klinger, Tyler Westover, and Sheng Dai. 2021. "Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model." *Powder Technology* 383: 396–409. https://doi.org/10.1016/j.powtec.2021.01.027.

Open-Source Flow Simulation Toolkits

Task 3 researchers completed the open-source release of three separate code bases, making them freely available to external stakeholders.[14] These codes include **Granular Flow Models**: user-defined material behavior description subroutines for the computational fluid dynamics modeling package Abaqus; **densegranFoam**: an OpenFOAM computational fluid dynamics model for dense granular material flow; and **LIGGGHTS-INL**: an extended version of the LIGGGHTS open-source discrete element method particle simulation software. These experimentally validated computational models will enable sophisticated modelers in industry and academia to simulate the flow behavior of biomass feedstocks with properties very different from traditional agricultural commodities.

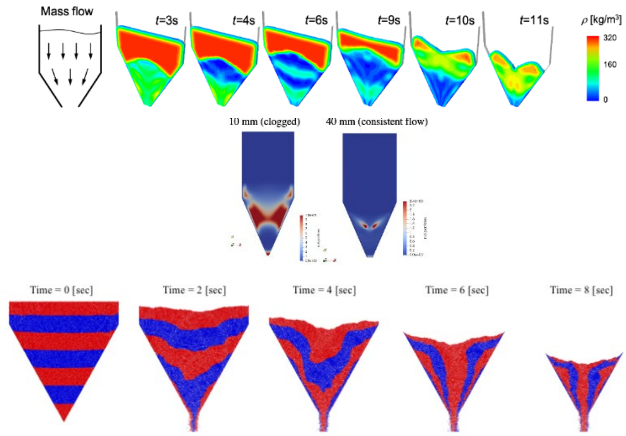

Figure 9. Open-source biomass flow modeling tools can predict complex biomass flow behavior in hoppers and bins.

Design Heuristics for Industry

Detailed parametric studies, using both the advanced modeling[15,16,17] and experimental efforts described above, were performed to develop design charts that predict the critical hopper opening for dry pine chips flowing in (1) conical hoppers and (2) wedge-shaped hoppers. These charts can be used by process engineers to avoid undesirable conditions such as funnel flow or even flow stoppage caused by biomass arching in the hoppers.

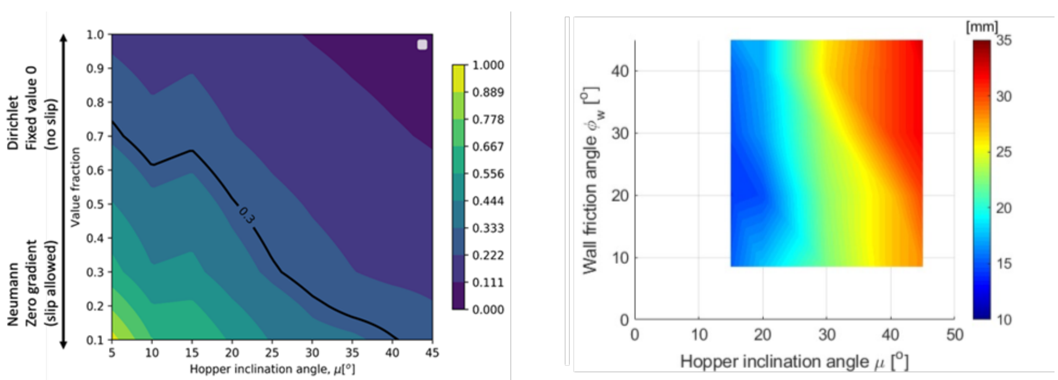

Figure 10. Open-source biomass flow modeling tools can predict complex biomass flow behavior in hoppers and bins.

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[14] GitHub repositories for open-source code are available at https://github.com/idaholab/GranularFlowModels (Granular Flow Models); https://github.com/NREL/densegranFoam; (densegranFoam); and https://github.com/idaholab/LIGGGHTS-INL (LIGGGHTS-INL).

[15] Yuan Guo, Qiushi Chen, Yidong Xia, Jordan Klinger, and Vicki Thompson. 2021. "A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles." *Powder Technology* 385: 557–571. https://doi.org/10.1016/j.powtec.2021.03.008.

[16] Yidong Xia, Feiyang Chen, Jordan Klinger, Joshua Kane, Tiasha Bhattacharjee, Robert Seifert, Oyelayo O. Ajayi, and Qiushi Chen. 2021. "Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation." *Biosystems Engineering* 205: 187–211. https://doi.org/10.1016/j.biosystemseng.2021.03.007.

[17] Yuan Guo, Qiushi Chen, Yidong Xia, Tyler Westover, Sandra Eksioglu, and Mohammad Roni. 2020. "Discrete element modeling of switchgrass particles under compression and rotational shear." *Biomass and Bioenergy* 141: 105649. https://doi.org/10.1016/j.biombioe.2020.105649.

FY 2022 Goals

In FY 2022, Task 3 researchers will continue their work on first-principles-based modeling tools to predict the bulk flow of biomass feedstocks. Key outputs will include continuing to develop and validate models for estimating frictional forces in biomass feedstocks such as pine residues and corn stover.

Task 4 – Scientific Data Management

The objective of the Scientific Data Management task is to provide a collaborative computational environment for hypothesis development, experimental and modeling workflow management, integration of data sets 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)[18] and to enable easy collaborations among tasks using the open-source LabKey™ environment.

FY 2021 Key Results

Quality-by-Design Database in LabKey

A new tool on the FCIC Data Hub enables users to rapidly compose variations of bioenergy technology pathways from a standardized collection of unit operations linked to FCIC experimental data, and to render the pathways in diagrams that may be easily shared online with industry stakeholders. BETO-funded R&D teams still rely heavily on one-off spreadsheets or PDFs to share data, which saddles stakeholders with the chore of extracting and integrating such data offline. This new tool organizes and presents biorefinery designs, unit operations, and performance data within a standardized QbD framework. Industry stakeholders save time by viewing and downloading FCIC data that have been made findable, accessible, interoperable, and reusable (FAIR).

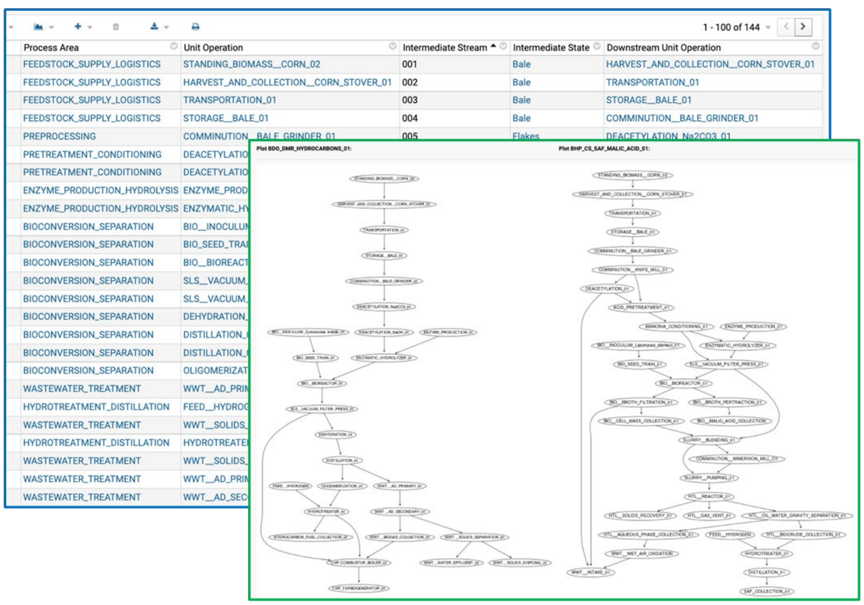

Figure 11. A new tool allows FCIC researchers to rapidly compose multiple variations of a given bioenergy conversion pathway and visualize the results quickly and easily.

FY 2022 Goals

In FY 2022, 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, and continuing to update the FCIC Data Hub web portal with curated data sets and publications.

[18] https://www.go-fair.org/fair-principles/

Task 5 – Preprocessing

The objective of the Preprocessing task is to develop 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 material attributes of corn stover and pine residues and process parameters of milling and deacetylation produce feedstocks with quality attributes required by downstream conversion.

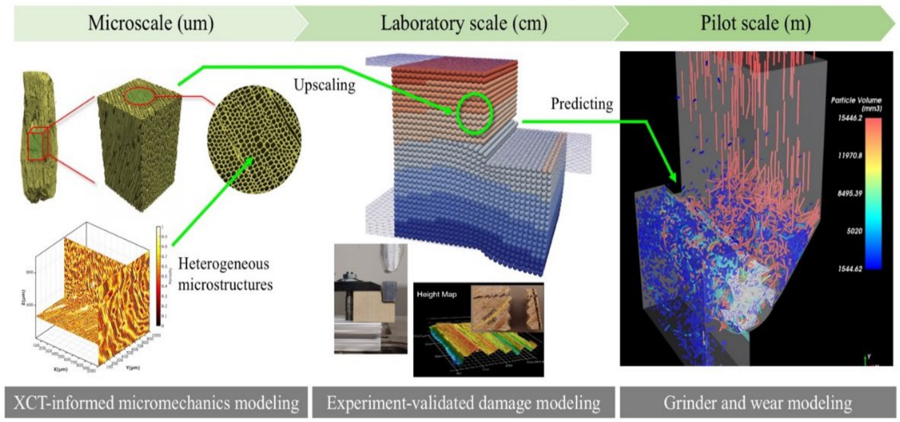

Figure 12. Preprocessing research spans multiple length scales and connects intrinsic biomass properties with comminution and deconstruction performance.

FY 2021 Key Results

Comminution Modeling

FCIC Task 5 developed a population balance model that predicts the milled particle size distribution of corn stover as a function of the corn stover initial particle size distribution and moisture content and the knife mill tip speed, geometry, and screen size. The model, which links single particle behavior to multiple particle impacts during milling operations, was validated with robust experimental data. This modeling tool will allow biorefinery operators to move beyond "rules of thumb" and empiricism and will allow industrial-scale simulations to inform and optimize mill design and guide mill operations.

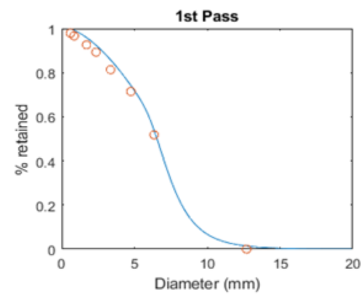

Figure 13. A population balance model predicts corn stover particle size distribution from feedstock and mill properties.

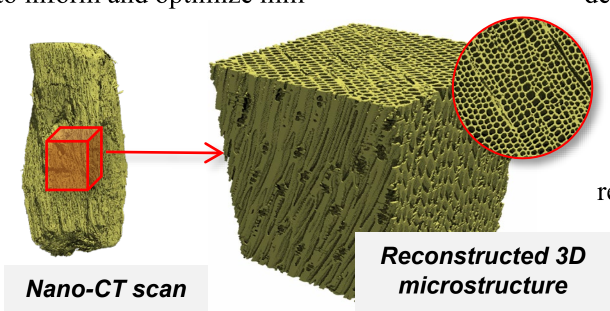

Figure 14. X-ray computed tomography scans of biomass can be reconstructed digitally as realistic structures for computational modeling.

Characterization of Microstructures

FCIC Task 5 researchers developed a method to reconstruct X-ray computed tomography scans to provide direct determination of realistic biomass microstructures[19] for subsequent modeling. The method allows the determination of envelope porosity, local porosity, and directional porosity, and results showed conclusively substantial heterogeneity in local and direction porosity at the microscale.

[19] Quan Sun, Yidong Xia, Jordan Klinger, Robert Seifert, Joshua Kane, Vicki Thompson, and Qiushi Chen. 2021. "X-ray computed tomography-based porosity analysis: Algorithms and application for porous woody biomass." *Powder Technology* 388: 496–504. https://doi.org/10.1016/j.powtec.2021.05.006.

Deacetylation Modeling

DMR is a low-temperature biomass deconstruction technique that leverages technology developed for pulp and paper manufacturing to produce cellulosic sugars that can be upgraded to a variety of biofuels and bioproducts.[20] Task 5 researchers designed and built a packed-bed flow column system with temperature control and pressure gradient measurement.[21] Using experimental data from this system, the researchers developed and validated a physics-based mechanistic model to predict permeability and flowability implications relevant to industrial processing and developed a compressible packed-bed model to allow the scale-up of the process to industrially relevant reactor sizes.

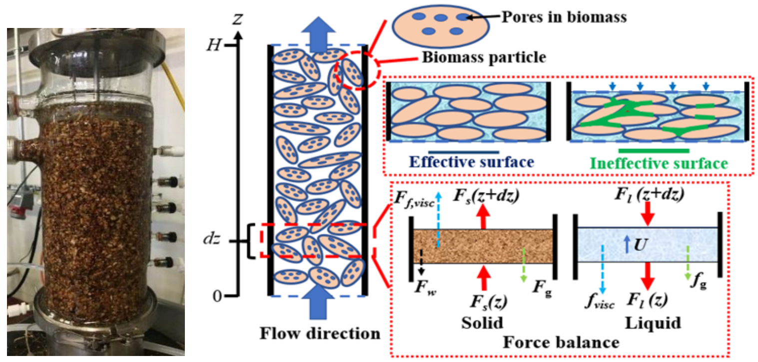

Figure 15. A laboratory-scale deacetylation reactor was designed and built to generate robust engineering data to validate a physics-based, mechanistic packed-bed hydrodyamic model useful for reactor scale-up.

Coarse-Grained Modeling of Lignocellulose Mechanics

Molecular simulations are providing fundamental knowledge about how forces at the molecular scale propagate through large lignocellulose structures. Lignocellulose is a complex intertwining of three biopolymers (cellulose, hemicellulose, and lignin). Lignin is a random polymer of different aromatic subunits, and the relative amounts of lignin subunits can vary markedly in different biomass types. It is not known how these ratios impact physical properties of lignocellulose. Molecular dynamics simulations clearly show that higher syringyl/guaiacyl (S/G) aromatic subunit ratios require more mechanical energy to deconstruct, suggesting that genetic engineering strategies might be able to produce specific biomass feedstock cultivars that minimize energy inputs in conversion processes.

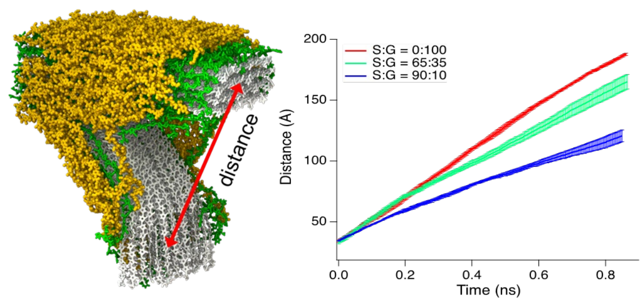

Figure 16. Molecular dynamics modeling show differences in biomass chemistry lead to differences in mechanical properties.

FY 2022 Goals

In FY 2022, Task 5 researchers will continue their combined experimental and modeling approaches to understand the impacts of feedstock variability on preprocessing of loblolly pine and corn stover and expand this work to look at MSW. The Task 5 researchers will also continue their real-time feedstock analysis and continue their multiscale particle modeling. In addition, they will build on their work in deacetylation and develop a high-throughput conversion screening assay to provide conversion performance data for the low-temperature pathway (DMR/enzymatic hydrolysis). This high-throughput conversion assay will provide critical information relating feedstock material attributes to conversion quality attributes and may eventually permit the prediction of conversion performance from feedstock material attributes alone.

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[20] Xiaowen Chen, Erik Kuhn, Edward W. Jennings, Robert Nelson, Ling Tao, Min Zhan, and Melvin P. Tucker. 2016. "DMR processing of corn stover achieves high monomeric sugar concentrations (230 g L^{-1}) during enzymatic hydrolysis and high ethanol concentrations (>10% v/v) during fermentation without hydrolysate purification or concentration." *Energy & Environmental Science* 9: 1257. https://doi.org/10.1039/c5ee03718b.

[21] Yudong Li, Xiaowen Chen, and David A. Sievers. 2021. "Modelling a compressible packed bed flow-through washing and deacetylation reactor for corn stover pretreatment." *Chemical Engineering Journal* 415: 128918. https://doi.org/10.1016/j.cej.2021.128918.

Task 6 – High-Temperature Conversion

The objective of the High-Temperature Conversion task is to develop the science-based understanding required to accurately predict the effects of variable feedstock attributes and process parameters on pyrolysis product quality attributes. The impacts of feedstock variability on high-temperature unit operations are either not known or poorly defined. Current design principles are based on empirically derived guidelines that are only useful over a very narrow range of feedstock properties and reactor types. The work from Task 6 will allow biorefinery designers and operators to design high-temperature unit operations/processes that are flexible and responsive to naturally occurring and market-dictated feedstock variability, while maximizing productivity. We aim to produce a validated, multiscale experimental and computational framework and high-throughput screening pipeline that allows biorefinery designers and operators to maximize productivity and intermediate product quality with variable incoming feedstock.

FY 2021 Key Results

Multiscale Modeling Framework

Task 6 researchers continued their work to build a multiscale modeling framework[22,23,24] to understand the impacts of feedstock material attributes on the quality attributes of the products from a fluidized-bed fast pyrolysis reactor. The multiscale aspect of this work is key because characterization of the critical material attributes that affect the overall reactor performance manifest themselves at different scales. The intrinsic kinetics are influenced by intra-particle heat and mass transfer limitations, so particle-scale modeling is necessary to elucidate these impacts. The heat and mass transfer limitations in the fluidized-bed pyrolyzer manifest themselves at the reactor scale, so a different modeling scale is necessary. Finally, a rapid approach to understanding the techno-economic implications of conversion data requires yet another type of modeling. The Task 6 team is integrating all these modeling approaches to provide stakeholders with actionable information on the impact of feedstock variability on high-temperature conversion performance.

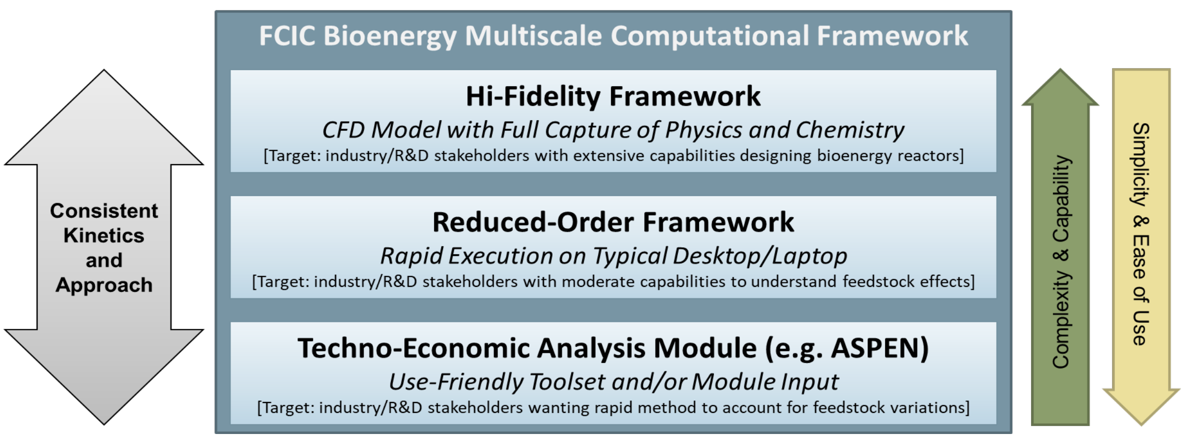

Figure 17. A validated, multiscale experimental and computational framework will enable biorefinery design engineers and operators to predict critical product quality attributes from variable feedstock critical material attributes.

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[22] Xi Gao, Liqiang Lu, Mehrdad Shahnam, William A. Rogers, Kristin Smith, Katherine Gaston, David Robichaud, et al. 2021. "Assessment of a Detailed Biomass Pyrolysis Kinetic Scheme in Multiscale Simulations of a Single-Particle Pyrolyzer and a Pilot-Scale Entrained Flow Pyrolyzer." *Chemical Engineering Journal* 418: 129347. https://doi.org/10.1016/j.cej.2021.129347.

[23] Liqiang Lu, Xi Gao, Aytekin Gel, Gavin M. Wiggins, Meagan Crowley, Brennan Pecha, Mehrdad Shahnam, William A. Rogers, James Parks, and Peter N. Ciesielski. 2021. "Investigating Biomass Composition and Size Effects on Fast Pyrolysis Using Global Sensitivity Analysis and CFD Simulations." *Chemical Engineering Journal* 421 (Part 2): 127789. https://doi.org/10.1016/j.cej.2020.127789.

[24] M. Brennan Pecha, Nicholas E. Thornburg, Chad A. Peterson, Meagan F. Crowley, Xi Gao, Liqiang Lu, Gavin Wiggins, Robert C. Brown, and Peter N. Ciesielski. 2021. "Impacts of Anisotropic Porosity on Heat Transfer and Off-Gassing during Biomass Pyrolysis." *Energy and Fuels* 35 (24): 20131–20141. https://doi.org/10.1021/acs.energyfuels.1c02679.

Experimental Validation of Conversion Modeling

While the multiscale modeling framework being developed by Task 6 researchers represents a very powerful set of tools for understanding the impact of feedstock variability on high-temperature conversion performance, the models must be developed and then validated with high-quality compositional analysis and experimental conversion data. Thanks to careful analytical chemistry using a variety of instrumental analysis techniques and laboratory experiments at multiple scales, the validated modeling framework has been demonstrated to predict the impact of biomass chemistry on pyrolysis oil yield within approximately 5%, and oil chemistry predictions similar to experimental trends.

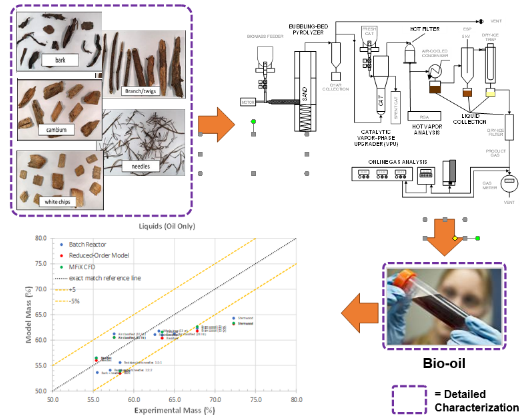

Figure 18. A multiscale modeling framework validated by robust experimental data helps stakeholders understand the impact of feedstock variability on high-temperature conversion performance.

Predicting Economic Impacts of Feedstock Variability

Task 6 researchers demonstrated the utility of the multiscale modeling framework by investigating the impacts of pine residue feedstock material attributes on catalytical fast pyrolysis conversion performance and subsequently the overall techno-economics of the process.[25]

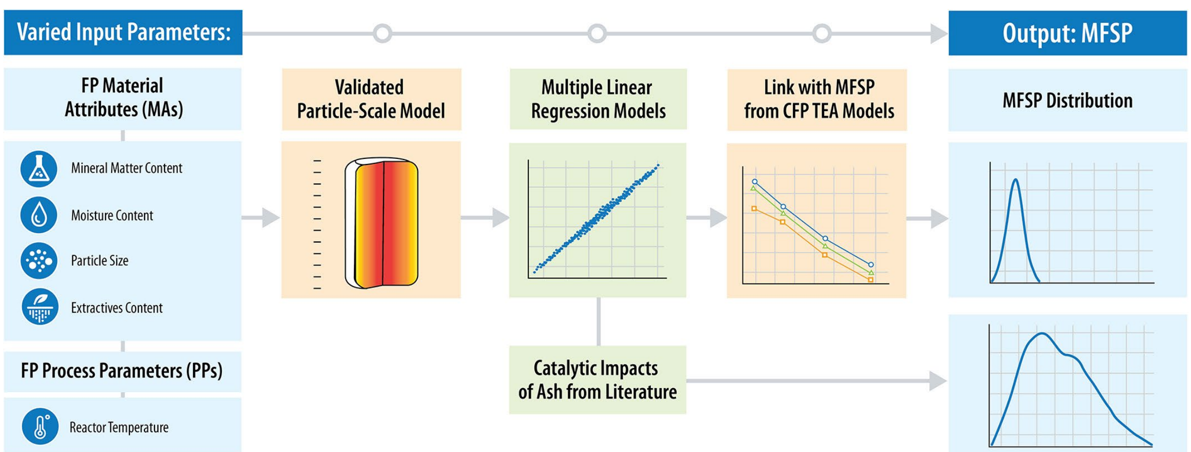

Figure 19. FCIC Task 6 researchers, in collaboration with Task 8 – Crosscutting Analyses, used the multiscale modeling framework to predict the impact of feedstock material attributes on the process economics of fast pyrolysis (from Wiatrowski et al. 2022).

FY 2022 Goals

In FY 2022, Task 6 researchers will continue their work to develop the science-based understanding of the effects of feedstock variability on high-temperature conversion. The capstone output of Task 6 will be the validation and integration of all results and models into a final experimental and computational framework that captures the fundamental physics and chemistry of biomass feeding and pyrolysis unit operations as a function of feedstock particle morphology, anatomical fraction, organic composition, and inorganic speciation. They will also extend the combined modeling and experimental approach to include gasification, add representative MSW materials as feedstocks, and continue work on quantitative chemical characterization approaches to measure the processability of pyrolysis bio-oils in downstream hydrotreating or co-processing applications.

[25] Matthew R. Wiatrowski, Abhijit Dutta, M. Brennan Pecha, Meagan Crowley, Peter N. Ciesielski, and Daniel Carpenter. 2022. “A simplified integrated framework for predicting the economic impacts of feedstock variations in a catalytic fast pyrolysis conversion process.” *Biofuels, Bioproducts, and Biorefining* 16 (2): 403–412. https://doi.org/10.1002/bbb.2319.

Task 7 – Low-Temperature Conversion

The objectives of the Low-Temperature Conversion task are to determine the effects of biomass feedstock variability on unit operation required for low-temperature conversion processes (utilizing both sugar and lignin pathways) and to develop tools to mitigate the risks posed by this variability. The interdisciplinary research team in Task 7 is uncovering knowledge and developing tools that minimize the impacts of feedstock and process variability on microbial conversion performance so that we can operate the sequential cascade of low-temperature processes intelligently by understanding critical attributes of materials passed downstream and by adjusting process parameters that allow for tolerance of upstream complications. 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 2021 Key Results

Feedstock Variability Affects Bioconversion Processes

There are limited public data regarding the impact of feedstock variability on organism performance in fermentors using sugar and lignin streams derived from biomass subjected to deacetylation,mechanical refining and enzyme hydrolysis. FCIC researchers observed statistically significant changes in both deconstruction performance and subsequent biocatalytic productivity and substrate utilization for corn stover feedstocks of varying quality. Strikingly, conversion performance was impacted for both the sugar- and lignin-converting organisms, but with differing effects on the processes. These results are the first of their kind to determine, in a controlled manner, the effects of feedstock variability on the biological conversion performance of DMR-pretreated feedstock streams.

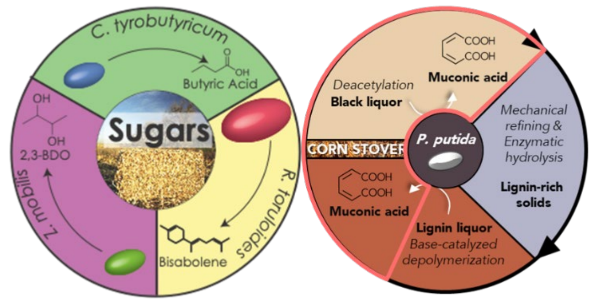

Figure 20. DMR/EH pretreatment results in a sugar-rich hydrolysate as well as a lignin-rich liquor. FCIC researchers are investigating how feedstock variability impacts microbial conversion performance for both streams.

Deconstruction Process Modifications Do Not Impact Biocatalysis

A standard deconstruction process was deployed by Task 7 with modifications to improve potentially both process economics and sustainability metrics. Here, sodium carbonate was examined as a partial substitute for sodium hydroxide used in deacetylation. Task 7 researchers demonstrated that enzymatic hydrolysate generated from Na_2CO_3-mediated deacetylated material was utilized as efficiently by *Clostridium* (*C.*) *tyrobutyricum* as traditional NaOH-mediated deacetylated material (Figure 21), suggesting sodium carbonate substitution is a viable approach for improving both economic and environmental contributions.

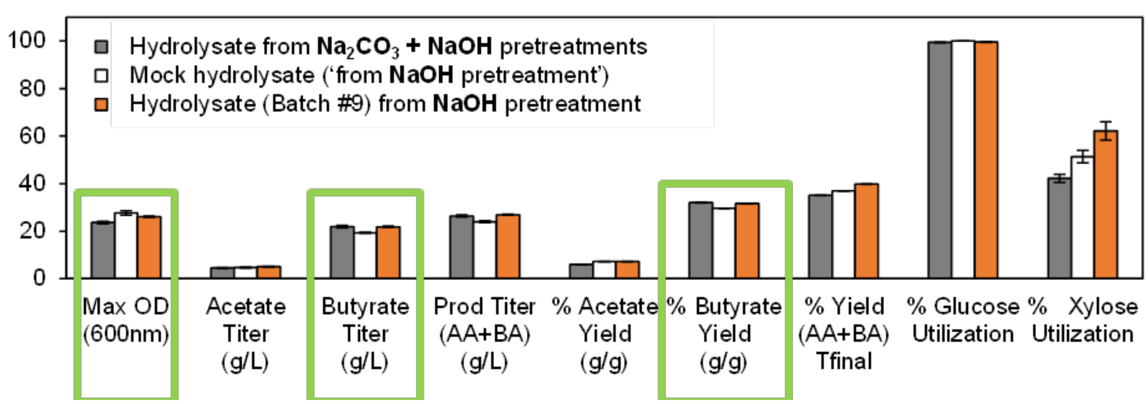

Figure 21. Partial substitution of sodium carbonate (Na_2CO_3) for sodium hydroxide (NaOH) during biomass deacetylation does not affect hydrolysate utilization by *Clostridium tyrobutyricum*.

Deconstructed Feedstocks May Need Less Preparation

The DMR-based deconstruction includes a comprehensive washing step. This wash removes the liquid phase—called black liquor—to recover unused caustic as well as prevent potentially inhibitory species in the black liquor from negatively impacting the enzymatic hydrolysis and biocatalytic upgrading. However, these inhibitory effects of the black liquor have not been investigated systematically. Task 7 researchers used high-throughput growth experiments to show that up to 20% black liquor can be tolerated in the enzymatic hydrolysate without any substantial decrease in *C. tyrobutyricum* biocatalytic performance (Figure 22).

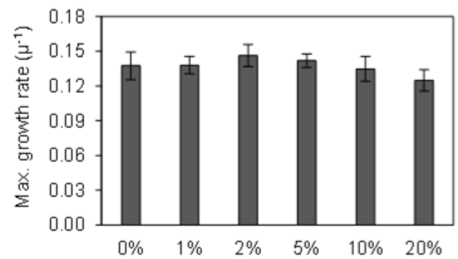

Figure 22. Black liquor (up to 20% v/v) does not affect *C. tyrobutyricum* growth rate.

Continuing Development of the Machine-Learning Framework

Machine-learning tools used both no-cost literature information and results obtained by the experimental teams to identify the material attributes and process parameters that impact low-temperature conversion. An opportunity existed to understand the genetic basis for tolerances and susceptibilities that were uncovered. Here, influences exerted by characteristics of raw materials and feedstock streams on the biocatalytic processes—whether similarly or differentially—could be understood on a first-principles basis by leveraging existing metabolic and regulatory models for the organisms comprising the training data set (Figure 23).

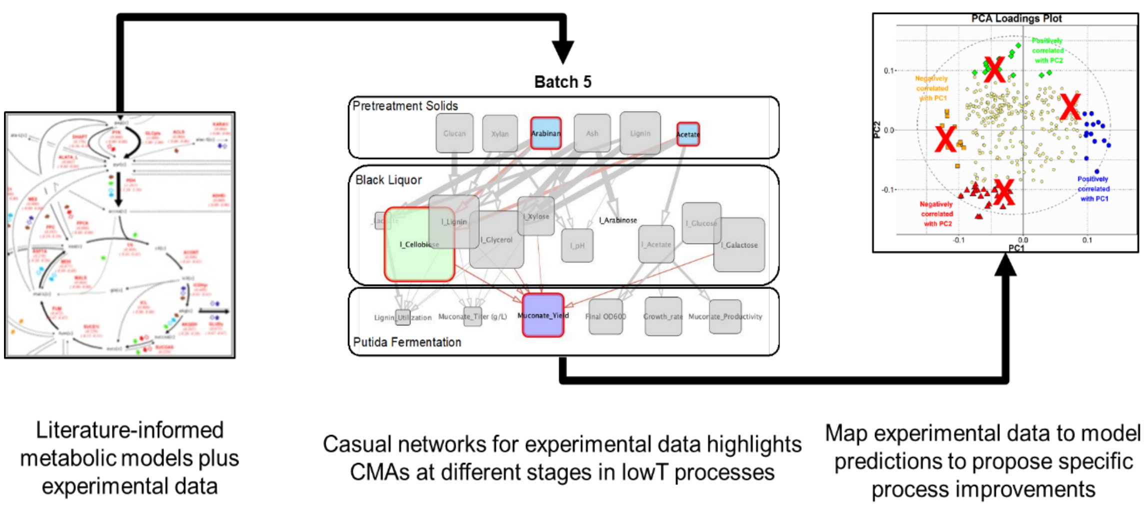

Figure 23. A machine-learning modeling framework combines literature and experimental data to identify the material attributes and process parameters that impact low-temperature biocatalytic conversion performance.

FY 2022 Goals

In FY 2022, Task 7 researchers will continue their interdisciplinary approach to determine the impact of biomass feedstock variability on the low-temperature conversion process chain. They will be investigating additional pretreatment chemistries to complement the work done with DMR to determine the effect(s) of both variable corn stover feedstock properties and variable deconstruction processes on downstream bioconversion performance. These data will be used 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 resources[26] 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 will (1) allow industry stakeholders to quickly understand both the economic sustainability implications of feedstock variability for specific unit operations and at a systems level, and (2) focus ongoing FCIC research efforts to address areas where feedstock variability is most impactful.

FY 2021 Key Results

Protected Storage for Corn Stover Bales Improves Quality

Protected storage using either tarped or covered storage can be justified with minor improvements in preprocessing costs or improved yields due to decreased dry matter loss and improved stover quality downstream. Protecting corn stover bales with tarps adds $1–$2/dry ton, and using a covered storage shed adds ~$10/dry ton to the delivered feedstock cost compared to uncovered storage. The additional cost of shed storage can be offset by as little as a ~2% increase in the carbohydrate content of the delivered feedstock.

Impact of Cut Height on Corn Stover Feedstock Costs

Harvesting corn stover at a higher position on the stalk (above lowest cob) removes less material than cutting lower (6 inches above ground). Because of the reduced stover removal and the increased transport costs, the high-cut stover is ~30% more expensive. The high-cut stover is enriched in cob and husk, which have been demonstrated to be less recalcitrant to downstream pretreatment. In addition, there may be sustainability benefits to removing less corn stover per acre.

Sorting Pine Residues at the Landing

Adding an in-field sorting step after mature pine tree harvesting increases the delivered cost of the biomass by up to 20% (based on representative literature data) but may provide higher-quality biomass feedstock for downstream conversion steps.

Saving Energy by Fractionating Corn Stover Prior to Milling

A substantial decrease in energy usage during hammer-milling corn stover offsets the additional costs associated with air classification; the air classification "pays for itself" in milling costs, not (yet) considering downstream costs.

Material Coatings Decrease Hammer Wear

Improving the wear rate of hammers (either by improved materials of construction or application of surface coatings) can provide an economic benefit under some circumstances. The "break-even" cost for improving hammer life is approximately 1.2 times the improved lifetime; for example, a twofold increase in hammer life at less than a 2.4-fold cost increase is beneficial. Improved hammer lifetimes up to a factor of 3 are useful; after this, other failure modes dominate the preprocessing costs.

Air Classification of Forest Residue for Tissue and Ash Separation Efficiency

Air classification of pine residues reduces the delivered cost of feedstocks by up to 5% by separating extrinsic (soil-derived) ash and bark and needles from logging residues and white wood for high-temperature conversion.

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[26] https://bioenergymodels.nrel.gov/models

Wet-Milling Pine Residues Reduces Fines and Ash and Saves Energy

Hammer milling in the pellet and feed industries is typically done with pre-dried feedstock, which minimizes grinding energy but leads to the generation of fines. While these fines are not of concern for pelleting operations, they may cause problems in high-temperature biomass conversion operations such as catalytic fast pyrolysis. Grinding pine residues prior to drying decreases the fines generated and leads to a greater fraction of the feedstock with lower ash content. The required drying energy is also substantially reduced compared to the conventional approach, leading to a threefold decrease in the carbon intensity of the process, as estimated by the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model.

Fermentation Impacts on Inorganic Compounds from Upstream Processing

High-throughput laboratory-scale growth experiments identified the inorganic compounds that may be present in industrially relevant corn stover hydrolysates. The reduced growth rate data translated to decreased productivity and therefore higher costs. The lignin upgrading pathway was more sensitive than the sugar upgrading pathway.

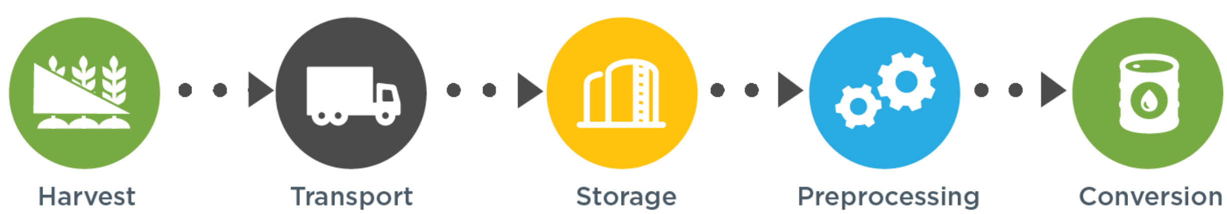
Isolated Anatomical Fractions of Corn Stover Convert Differently

The key anatomical fractions of corn stover (cobs, husks, stalks) showed substantially different low-temperature conversion performance in deacetylation followed by mechanical refining (DMR/enzymatic hydrolysis). These differences in the conversion performance of the fractions (cobs and husks were more reactive than either separated stalks or unseparated material) result in differences in estimated fuel costs. This work suggests that differential deconstruction of the individual fractions might result in improved overall systemwide costs and sets boundaries for the cost of separation of the fractions.

FY 2022 Goals

In FY 2022, 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 15 additional case studies are planned for FY 2022, 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), public webinars, conference presentations, and trade journals.



Directed Funding Opportunities (DFOs)

The FCIC awarded several cost-shared defined funding opportunities (DFOs) to enable FCIC researchers to work directly with industry partners to address specific industry concerns. While the technical details of these projects are protected by cooperative research and development agreements (CRADAs), the overall goals and outcomes of these projects provide a useful perspective on how FCIC researchers can work with industry partners.

Forest Concepts/Oak Ridge National Laboratory/Argonne National Laboratory

Forest Concepts (https://forestconcepts.com/) has developed a novel comminution system—the Crumbler® rotary shear—which produces biomass feedstocks with narrower particle size distribution, lower particle aspect ratio, and fewer fines than other comminution techniques such as hammermills or tub grinders. The goals of this project are to gain mechanistic insights for the wear issues experienced by the Crumbler rotary shear comminution system to provide combined materials and design solutions to improve the tool lifetime and processing, and to share these results broadly with the biomass industry.

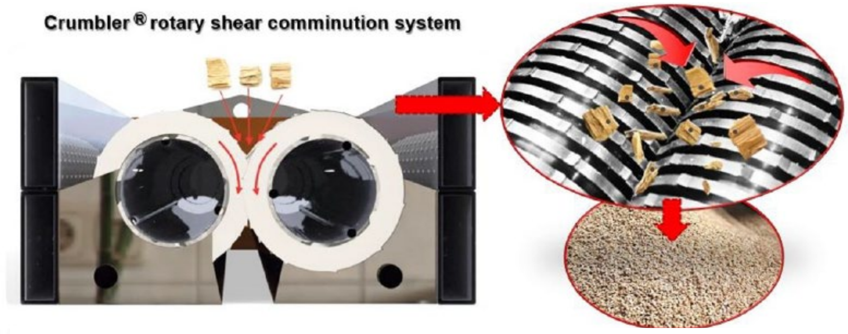


Figure 24. The Forest Concepts Crumbler rotary shear produces biomass feedstocks with narrow particle size distributions.

Fulcrum Energy/Idaho National Laboratory

Fulcrum Bioenergy (https://fulcrum-bioenergy.com/) uses gasification followed by Fisher-Tropsch synthesis to produce synthetic crude oil (syncrude) from MSW. They recently completed the Sierra BioFuels plant near Reno, Nevada, capable of processing 175,000 tons/year of MSW. The variability in the physical and mechanical properties of MSW represents an undesirable risk for the Fulcrum process. The overall objective of this project is to develop mechanical preprocessing technologies to densify the MSW and decrease the variability of its physical properties. The specific technical goals are to increase MSW density and reduce moisture to meet gasifier infeed requirements (e.g., moisture ~10%, bulk density ~480 kg/m^3, and durability >95%), while reducing the preprocessing cost by 40% as compared to conventional pelleting methods.

Figure 25. Pelletization of shredded MSW produces a densified material with reduced physical and mechanical variability.

Idaho Forest Group/Idaho National Laboratory

Idaho Forest Group (https://ifg.com) is an integrated company that grows, harvests, manufactures, and distributes sustainable wood products. The goal of this project is to improve the operational reliability and drying efficiency of low-temperature biomass dryers used by Idaho Forest Group by implementing real-time moisture sensors and adaptive process control strategies developed by INL researchers. When successful, the control system should reduce the variability in the moisture content of biomass exiting the dryer, improving product quality and increasing the operational reliability of the process.

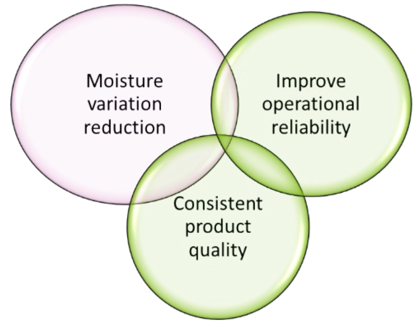


Figure 26. Adaptive process control algorithms can reduce the variability of sustainable wood products.

Jenike & Johanson/Los Alamos National Laboratory/Idaho National Laboratory

Jenike & Johanson (https://jenike.com) is the world's leading bulk material engineering firm, with expertise in power and bulk solid storage, handling, conveying, and processing. The objective of this project is to combine Los Alamos National Laboratory's expertise in acoustic sensing with Jenike & Johanson's expertise in solids handling to develop innovative "smart chute" material handling equipment and real-time monitoring of plug-screw feeder condition to improve the operational reliability, safety, throughput, and yield of biorefineries.

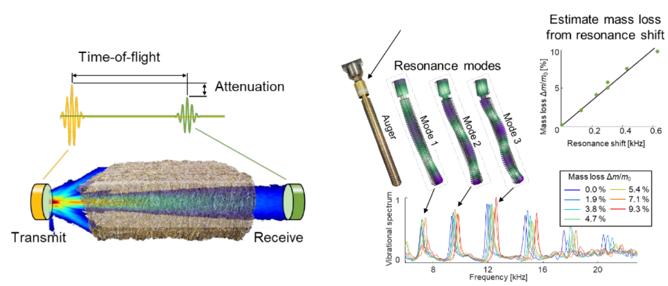


Figure 27. Low-cost acoustic sensing can characterize the moisture content of corn stover and wear characteristics of feed screws.

The Wonderful Company/National Renewable Energy Laboratory/Idaho National Laboratory/Jenike & Johanson

The Wonderful Company (https://www.wonderful.com) is the world's largest almond and pistachio grower, generating 250,000 tons of nut waste per year (wood, hulls, and shells). Fewer markets for these waste streams and new regulations regarding disposal has The Wonderful Company (and the rest of the industry) exploring opportunities to convert this waste stream into carbon-negative revenue via reliable electricity and bio-char production. The Wonderful Company is exploring gasification of their waste stream using systems designed and built by V-Grid Energy Systems (Camarillo, California). These systems generate electricity as well as biochar, a potential soil nutrient source. Researchers from the National Renewable Energy Laboratory and Idaho National Laboratory partnered with The Wonderful Company, V-Grid, and Jenike & Johanson (Tyngsboro, Massachusetts) to understand the impacts of waste attributes on conveyance and gasifier feeding, characterize the variability in these attributes, provide design guidance for reliable feeding systems, and demonstrate extended operation of an optimized system.

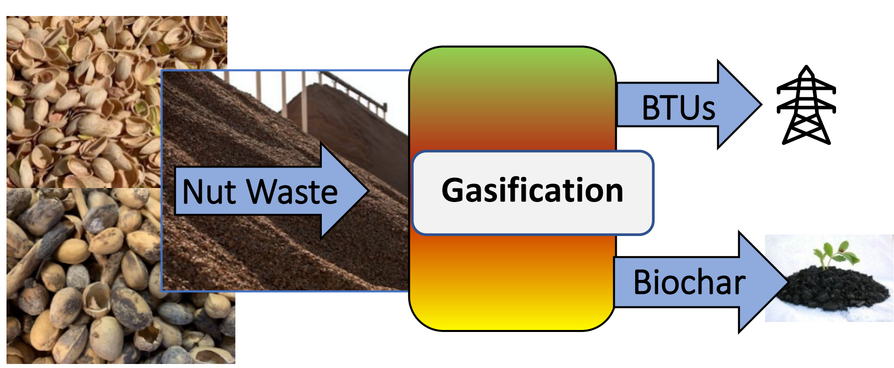


Figure 28. Characterizing the physical and mechanical properties of agricultural wastes such as pistachio shells is necessary to design low-cost and reliable handling and conversion technologies.

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