

FCIC Capstone Report

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About the FCIC

The Feedstock–Conversion Interface Consortium (FCIC), led by the U.S. Department of Energy’s (DOE’s) Bioenergy Technologies Office (BETO), is a collaborative effort among researchers from nine national laboratories focused on solving challenges related to biomass feedstock variability in biorefineries.

Researchers from the FCIC recognize that lignocellulosic feedstocks are nonhomogeneous and have greater variability compared to other agricultural commodities such as grains. As a result, empirical approaches to equipment design for processing these feedstocks have proven unsuccessful in pioneer biorefineries.

FCIC researchers use first–principles–based science to better understand the physical, mechanical, thermochemical, and biochemical interactions and reactions as solid feedstocks are processed in biorefineries to produce liquid fuels and bioproducts. This knowledge is used to develop models and tools that help industry de–risk biorefinery scale–up and deployment and optimize bioenergy conversion processes in the future.



Introduction

The inherent variability of the physical, chemical, and mechanical attributes of biomass poses substantial challenges to the scale-up and commercialization of promising technologies that use biomass resources to produce sustainable fuels, chemicals, and materials in the emerging bioeconomy.¹ Managing this variability is critical to ensuring the reliable performance, economic viability, and sustainability of these technologies.

A single biomass feedstock, such as corn stover, can exhibit wide variations in physical, chemical, and mechanical attributes such as composition, convertibility, or bulk density across individual samples. These differences are even more pronounced between different biomass types. For example, agricultural residues such as corn stover differ substantially from forestry residues and from purpose-grown crops such as switchgrass or miscanthus. In addition, the attributes of biomass feedstocks are greatly influenced by how they are harvested, transported, stored, and processed. Because these attributes directly impact the value of the biomass to biorefineries, managing this variability is critical.

Unlike familiar agricultural commodities such as corn, wheat, and barley—which have been processed at industrial scales for more than 100 years and at smaller scales for millennia—lignocellulosic feedstocks exhibit unique properties that make them more challenging to handle. Figure 1 illustrates the intrinsic variability of biomass: pine residues, for example, have distinct anatomical fractions such as bark, needles, and stem wood, whereas corn stover has distinct anatomical fractions including cobs, husks, and stalks, each with different attributes. In addition, changes to the biomass can occur over time. Improper storage can lead to moisture-induced degradation and cause substantial changes in the biomass. Because of these complexities, attempts to adapt traditional grain-processing equipment to handle biomass have proven unsuccessful, underscoring the need for new solutions to process biomass effectively at scale.

BETO has established strategic goals² to decarbonize the transportation, industrial, and agricultural sectors to move the United States into a more sustainable future and a robust bioeconomy

¹ Biorefinery Optimization Workshop Summary Report. DOE/EE-1514 (December 2016). <https://www.energy.gov/eere/bioenergy/downloads/biorefinery-optimization-workshop-summary-report>.

² Bioenergy Technologies Office Multi-Year Program Plan. DOE/EE-2698 (March 2023). <https://www.energy.gov/sites/default/files/2023-03/beto-mypp-fy23.pdf>.

is critical to achieve these goals. Biomass feedstock variability is recognized as a key contributor to the failure of multiple pioneer biorefinery projects in the last decade¹ and continues to represent a substantial risk to the scale-up and deployment of next-generation bioenergy technologies. BETO formed the FCIC to reduce this risk and to enable the rapid growth of the bioeconomy.

The FCIC brought together a large team of researchers with many different areas of expertise equipped with the extensive experimental and computational resources of 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
- Sandia National Laboratories.

BETO recognizes that although the FCIC member laboratories will not design or operate next-generation biorefineries, the FCIC can develop first-principles-based knowledge and tools that industry stakeholders can use to address known issues associated with feedstock variability during the design and operation of these biorefineries. The interdisciplinary FCIC team was therefore challenged to address the pressing issue of biomass feedstock variability across the entire bioenergy value chain using their deep subject matter expertise and the unique experimental and computational resources of the national laboratories.

The FCIC has met this challenge and has made an array of knowledge and tools available to industry stakeholders in the form of publicly available scientific publications, technical reports, conference presentations, and open-source computer codes available for download. BETO believes that the success of this consortium will be measured by how the tools and knowledge generated by FCIC researchers are used to de-risk biorefinery scale-up and prevent future scale-up failures.

Industry interest and engagement are additional measures of success of the FCIC. Researchers from the FCIC have collaborated with 11 companies through BETO-funded Cooperative Research and Development Agreement (CRADA) projects and have had numerous informal conversations with

industry stakeholders. The defined funding opportunity issued in 2023³ was oversubscribed by a factor of 4 compared to the available budget. Because of this overwhelming industry interest, an Industry Partnership Call has recently been released.⁴

Industry interest and appreciation for the FCIC are evident in quotations from some of our industry partners:

“Our company has always wondered how certain feedstock properties impact our gasification process. The FCIC program gave us the unique opportunity to work with [the National Renewable Energy Laboratory (NREL)] to explore that more deeply. The project enables us [to] use world-class facilities and experts for an important problem, but we most value the long-term relationships it helps to develop.”

“We really value the partnership we developed with [the Oak Ridge National Laboratory, (ORNL)] as part of the FCIC program. Typically a small business like ours would not have access to this depth of expertise or the world class analysis equipment. Partnering with a national lab allowed us to explore solutions in a more complete method.”

“FCIC has been instrumental in our journey into de-risking and establishing [municipal solid waste, (MSW)] project models. Their work provides invaluable early insight into project design, while bringing together multiple scientific and industry partners. The FCIC’s ability to enable these partners to work together and provide subject matter expertise across a broad range of disciplines is essential for achieving success in as complex a model as biofuels from [MSW].”

“Our technology has a huge promise to address the world’s third-largest [methane emissions source]. Having ORNL work closely [with us] will be absolutely critical for us.”

The achievements of the FCIC are summarized only briefly in this report. Details are presented in more than 100 scientific publications, conference presentations, and technical reports, links to which are included at the end of this report.



Figure 1. Feedstocks are intrinsically variable. (A) Pine residues have distinct anatomical fractions, including (L-R) bark, needles, stem wood, and whole material. (B) Corn stover anatomical fractions are also distinct and include (L-R) whole stover, cobs, husks, and stalks. (C) A single bale of corn stover can have widely varying amounts of moisture-induced degradation resulting from improper storage.

³ <https://www.energy.gov/eere/bioenergy/fcic-cooperative-research-and-development-agreement-call>

⁴ <https://www.energy.gov/eere/bioenergy/us-department-energy-selects-seven-projects-help-industry-leverage-fcic-capabilities>





Objectives, Organization, and Approach

The objective of the FCIC was to reduce the scale-up risks biorefineries face because of feedstock variability. To achieve this, FCIC researchers shifted from the traditional paradigm of feedstock variability, in which feedstocks were classified primarily by name and feedstock properties such as composition, moisture and ash content, and mean particle size. In the new paradigm, first-principles science replaced empiricism. Feedstock variability is now understood in terms of the physical, chemical, and mechanical attributes of the biomass and the ways these attributes change across the bioenergy value chain.

Research by the FCIC focused on three model feedstocks representing woody biomass, herbaceous biomass, and waste materials. Pine residues, sourced from both whole-tree thinning operations and timber harvest activities, were used as a model for woody residues. Residue from thinning operations consists of immature whole trees removed to improve forest health, whereas timber harvest residues are the portion of the mature trees not used for lumber such as

tops, branches, and bark. Corn stover, the portions of the plant left after removing the grain, served as a model for agricultural residues. As a model for waste material, landfill-bound residues from a material recovery facility (MRF) were used as an example of widely available and potentially valuable solid waste.

FCIC researchers worked with biomass samples selected to show naturally occurring variability. Whole-tree thinnings and timber harvest residues represented two different potential sources of pine residue. Multiple corn stover samples were collected with known differences in composition, including samples that had undergone significant drought stress during growth and samples that had undergone biological degradation because of inappropriate storage. These samples provided a snapshot of some of the natural and process-induced variability present in biomass.

Sample tracking was an essential component of robust research. The Idaho National Laboratory's (INL's) Bioenergy Feedstock Library⁵ (BFL) was used

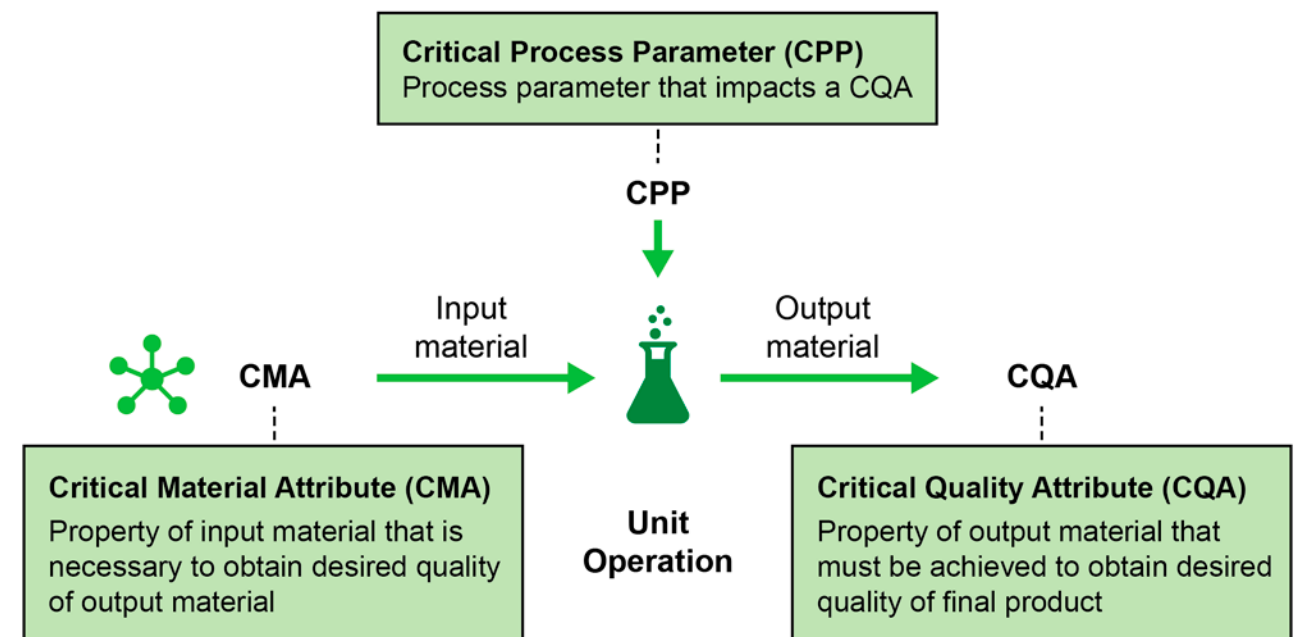


Figure 2. The QbD concept is a key organizing principle of the FCIC. Endorsed by the FDA and widely used in pharmaceutical manufacturing, it focuses on a fundamental understanding of individual unit operations and the interactions among the multiple unit operations that make up a bioenergy conversion process.

to track samples with unique identifier and parent/child relationships across the entire value chain, ensuring thorough documentation and traceability.

Quality by Design

The technical approach used by FCIC researchers was based on the “quality-by-design” (QbD) concept, originally developed by Dr. Joseph M. Juran and later adopted by the U.S. Food and Drug Administration (FDA), which oversees pharmaceutical manufacturing in the United States.^{6,7} The QbD concept builds on the concepts of total quality management and continuous quality improvement, which guide global manufacturing operations from electronics to automobiles to drugs. FCIC researchers have incorporated several key QbD principles in their research efforts.

First, FCIC researchers focused on developing a comprehensive understanding of individual steps in the bioenergy value chain—the unit operations—

based on fundamental scientific and engineering principles. Second, FCIC researchers investigated the performance of these unit operations in terms of the physical, chemical, and mechanical characteristics of the materials entering and leaving the unit operations, referred to as critical material attributes (CMAs) and critical quality attributes (CQAs), respectively, and the ways the unit operations are operated, referred to as critical process parameters (CPPs). Essentially, FCIC researchers moved the research discussion from feedstock and process **names** to feedstock and process **attributes**. Third, FCIC researchers examined system-level effects that arise as multiple unit operations interact and impact each other.

⁵ Idaho National Laboratory Biomass Feedstock Library. <https://bioenergylibrary.inl.gov/Home/Home.aspx>.

⁶ Yu, L. X., Amidon, G., Khan, M. A. et al. 2014. “Understanding Pharmaceutical Quality by Design.” *AAPS J* 16:771–783. <https://doi.org/10.1208/s12248-014-9598-3>.

⁷ Juran, J. M. 1992. *Juran on Quality by Design: The New Steps for Planning Quality into Goods and Services*. New York: Free Press.

Research Areas

Work within the FCIC spanned the entire bioenergy value chain: biomass feedstock characterization; material handling, preprocessing, equipment wear analysis; and low- and high-temperature conversion. The FCIC also supported efforts in cross-cutting analysis and data integration.

Although the research approaches in these different areas varied, some common themes are clear. First, **all research efforts required significant subject matter expertise**, necessitating an interdisciplinary approach. For example, the expertise required for metabolic modeling differed from that needed for wear analysis, but both skillsets were essential to the work of the FCIC. The broad range of experience within the FCIC's member national laboratories provided the diverse expertise necessary for these efforts.

Second, all research efforts also included a **substantial experimental component**. Robust experimental data are the foundation of good science, and the experimental facilities at the FCIC's member national laboratories enabled FCIC researchers to generate high-quality data. These data were essential not only for developing and validating computational models but also for addressing specific research questions directly.

Third, the research efforts included **extensive computational model development**. These complex and computationally intensive predictive models were developed using the high-performance computing (HPC) resources of the national laboratory system, based on first-principles science, and validated experimentally. These modeling efforts, along with the resulting modeling tools, offer multiple benefits. They help researchers understand the fundamental physics and chemistry of biomass conversion processes, and once validated, can be used to conduct virtual experiments that would be prohibitively expensive to perform in a laboratory or pilot plant. Most importantly, these models can be simplified for use by others without access to HPC resources and can be combined with techno-economic analysis (TEA) and life cycle analysis (LCA) models to quickly assess the economic and sustainability impacts of feedstock variability.

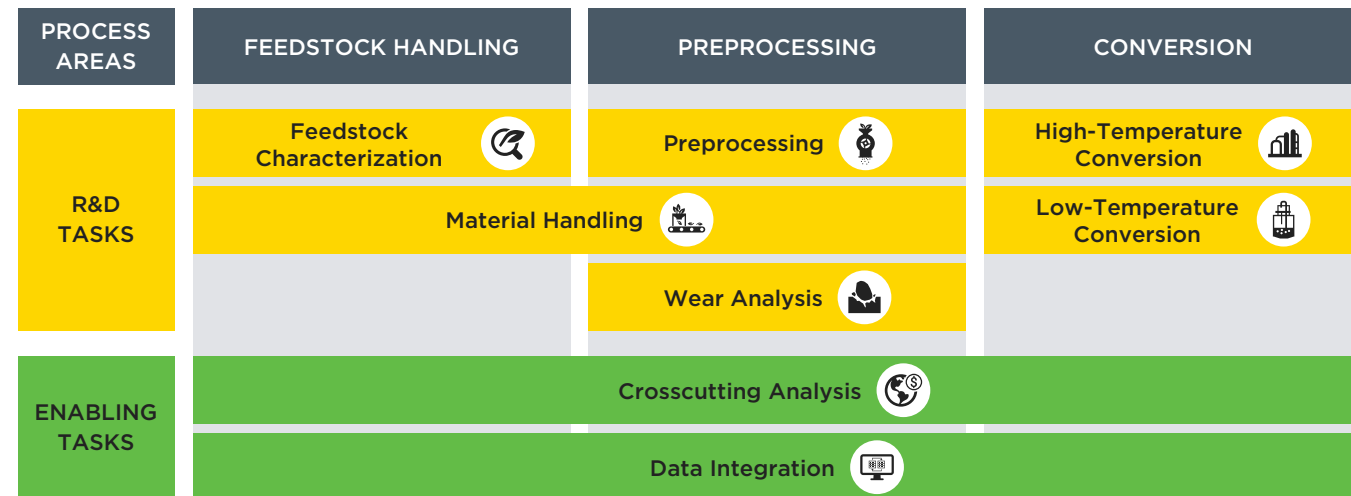


Figure 3. High-level organizational chart of FCIC research areas. Work within the FCIC focused on six experimental areas and was supported by work in two enabling areas.

Feedstock Characterization

OBJECTIVE: Identify and quantify the distribution of feedstock critical material attributes, both intrinsic and process-induced, to better understand their impact on biomass handling and conversion processes.

OUTCOME: FCIC researchers summarized learnings about the impacts of feedstock variability on preprocessing and conversion processes and identified sources, distributions, and potential mitigation strategies for downstream processing of corn stover, forest residues, and solid waste residues.

IMPACT: A better understanding of biomass feedstock variability provides actionable insights for industry stakeholders, informs best practices across the entire bioenergy value chain, and ultimately de-risks a key element of biorefinery scale-up.

The FCIC's **feedstock characterization** work focused on detailed analyses of biomass resources to understand their physical, chemical, and mechanical attributes that impact the bioenergy value chain. The work was successful, revealing that these feedstock attributes fall into only a few categories, each of which is now understood at a more fundamental level.

For example, better than simply knowing particle size is knowing critical attributes such as the particle size distribution (PSD), distribution of particle shapes, and particle densities and porosities. Similarly, more comprehensive than knowing the total ash content is identifying the specific inorganic species composing the ash, because different species affect different process steps in distinct ways. In addition, it is important to understand whether the inorganic species are intrinsic to the biomass material or introduced during processing because the former are much more difficult to modify than the latter.



FCIC researcher Bryon Donohoe from NREL used advanced analytical techniques like electron microscopy to investigate feedstock variability.

Old Paradigm	New Paradigm
Particle Size	<ul style="list-style-type: none"> Particle Size Distribution Particle Morphology Bulk Density Compressibility Toughness
Ash Content	<ul style="list-style-type: none"> Inorganic content Inorganic speciation Source(s) of added inorganics
Moisture Content	<ul style="list-style-type: none"> Harvest/storage/transport history Moisture-induced attribute changes
Additional physical, chemical, and mechanical attributes	

Table 1. The new paradigm for biomass characterization expands on the information previously considered to include a broader range of physical, chemical, and mechanical attributes.



FCIC researcher Tiasha Bhattacharjee from INL testing ring shear equipment. Careful experimental work revealed variability in biomass mechanical attributes, important details for predicting the flow and comminution properties of biomass.

Material Handling

OBJECTIVE: Develop first-principles-based design tools to enable trouble-free bulk flow of biomass materials that are practical for and applicable to industry stakeholders.

OUTCOME: FCIC researchers developed and shared experimentally validated predictive computational tools and design charts that can be used to understand and predict the flow of biomass residues with variable properties in wedge hoppers, a frequent failure point in solids handling.

IMPACT: Accessible design charts for biomass material flow in bins and hoppers and, more importantly, the tools that can be used to extend these results to similar equipment, move biomass handling predictions away from empiricism and toward more rigorous, first-principles-based science.

The objective of the FCIC's **material handling** work was to develop practical, applicable, and first-principles-based design tools to enable trouble-free bulk flow of biomass materials for industry stakeholders. The final milestone was to develop and share experimentally validated computational tools and design charts useful for predicting the flow of biomass residues with variable properties in wedge hoppers, a frequent failure point in solids handling.

The success of this work required the development of several computationally intensive models using the HPC capabilities of the national laboratories as well as a substantial amount of experimental data collected at multiple scales. The results of this modeling work have been published in numerous technical publications and presentations, and the modeling tools have been shared as open-source codes to help industry stakeholders effectively design equipment. An example of a design chart and a list of these open-source tools are included later in the report.

Preprocessing

OBJECTIVE: Develop first-principles-based design tools to understand and predict biomass comminution performance during preprocessing.

OUTCOME: FCIC researchers developed and shared experimentally validated, data-driven computational tools and design charts that predict the final output PSD for feedstocks with variable attributes and under variable operating conditions.

IMPACT: Detailed design charts for specific comminution equipment and, more importantly, the tools that can be used to extend these results to similar equipment move comminution performance predictions away from empiricism and toward more rigorous first-principles-based science.

The goal of FCIC **preprocessing** work was to create first-principles-based design tools for the prediction of biomass comminution (e.g., hammer or knife mill) performance during preprocessing. The team developed and shared experimentally validated computational tools and design charts that use variable feedstock attributes and knife mill operating conditions to predict the final output PSD.

Like the material handling work, this successful project required not only the development of computationally intensive models using national laboratory HPC resources but also a substantial amount of multiscale experimental data for model development and validation. The results of this work have been published in numerous technical publications and presentations, and the modeling tools have been shared as open source tools.



Representative waste materials such as residues from material recovery facilities were used in FCIC research.



FCIC researchers at ORNL used microscopy techniques to examine wear.

Wear Analysis

OBJECTIVE: Develop a systematic approach integrating material characterization, wear modeling, and laboratory testing to gain a deep understanding of the mechanisms of equipment wear during biomass preprocessing, and to develop analytical tools and models for predicting wear.

OUTCOME: FCIC researchers developed, validated, and then shared with industry stakeholders a methodology and decision matrix for mitigating equipment wear in biorefineries as well as guidance on economic implications of mitigation strategies.

IMPACT: A clear and comprehensive approach to mitigating wear impacts that is grounded in first-principles science provides industry stakeholders with the knowledge to cost-effectively address wear issues in process equipment, and substantially reduces operational risks due to equipment wear.⁸

The focus of the FCIC's **wear analysis** work was twofold: (1) to develop a systematic approach combining material characterization, wear modeling, and laboratory testing to gain a deep understanding of the mechanisms of equipment wear biomass preprocessing and (2) to develop analytical tools and models that can predict wear.

The project was a success: researchers generated and shared results in numerous technical publications and led two BETO-funded industry collaborations, which are shared later in this report. For a final milestone, the researchers summarized their overall approach by developing and sharing with industry stakeholders a robust methodology and decision matrix for mitigating equipment wear in biorefineries and guidance regarding the techno-economic implications of mitigation strategies.

⁸ Qu, Jun, Erin Webb. 2024. "Enhancing the Reliability and Efficiency of Biomass Preprocessing." Resource Magazine. Accessed December 1, 2024. bt.e-ditionsbyfry.com/publication/?i=835634&p=18&view=issueViewer.

High-Temperature Conversion

OBJECTIVE: Develop an experimentally validated and multiscale computational framework for predicting high-temperature conversion performance of fast pyrolysis and gasification that relates feedstock material attributes and conversion reactor operating conditions to conversion performance.

OUTCOME: The FCIC delivered validated computational-experimental frameworks that capture the effects of feedstock critical material attributes and critical process parameters, enabling accurate predictions of product critical material attributes for variable feedstock attributes and process conditions.

IMPACT: A dramatic reduction in the time, effort, and costs associated with the process scale-up of high-temperature conversion reactors. The FCIC's modeling frameworks enable virtual experiments to assess the impact of feedstock variability on both pyrolysis and gasification, as well as their broader techno-economic impacts.

The objective of the FCIC's **high-temperature conversion** work was to develop an experimentally validated and multiscale computational framework for predicting high-temperature conversion performance, culminating in a tool that captures the effects of feedstock variability and conversion reactor conditions on high-temperature reactor performance.

In this successful endeavor, FCIC researchers developed validated modeling frameworks using national laboratory HPC resources for the high-temperature conversion of pine residues and solid waste through both fast pyrolysis and gasification. The original work plan focused on only pyrolysis but grew to encompass gasification as well in response to a shift in industry needs. Like previous efforts, this work required both computational modeling and experimental work. These modeling frameworks can be used for virtual experiments on the impact of feedstock variability on both pyrolysis and gasification, as well as their overall techno-economic impacts.



FCIC researcher Oluwafemi Oyedemi performing dynamic image characterization to assess particle size and shape distributions of woody biomass, which are critical material attributes for modeling thermochemical conversion processes.



FCIC researchers Gyorgy Babnigg (left), Kyle Hall (middle) and Phil Laible (right) from Argonne National Laboratory (ANL) participate in data analysis to understand how feedstock variability can impact low temperature conversion.



Low-Temperature Conversion

OBJECTIVE: Integrate careful experimental work with advanced modeling techniques to develop a machine learning framework to predict the microbial conversion performance of cellulosic sugar and soluble lignin streams in the fermentation stage of the low-temperature pathway.

OUTCOME: The FCIC developed an experimentally validated machine-learning-based predictive modeling tool for the microbial conversion performance of industry-relevant organisms using biomass-derived substrates.

IMPACT: A predictive modeling tool that enables the rapid screening of new organisms on biomass-derived sugar and lignin substrates, substantially reduces the need for extensive and time-consuming experimental work, and can accelerate the development of new biological pathways to produce sustainable fuels and products.

The FCIC's **low-temperature conversion** work was focused on developing a machine learning framework to predict the microbial conversion performance of cellulosic sugar and soluble lignin streams in the fermentation stage of the low-temperature pathway. The result was the successful creation of an experimentally validated machine-learning-based predictive modeling tool for the microbial conversion performance of industry-relevant organisms using biomass-derived substrates.

The work effectively used machine learning to integrate experimental datasets and complex metabolic models to build a predictive tool for the microbial conversion of biomass-derived sugar and lignin streams. The researchers noted a lack of substantial variability in the experimental microbial conversion performance data. Although different corn stover feedstocks provided different compositions of sugar and lignin substrates after the deacetylation and mechanical refining and enzymatic hydrolysis (DMR/EH) process, the organisms studied in the microbial conversion step were robust enough to deliver similar results for these different substrates. The minimal sensitivity to differences in these substrates suggests that **microbial conversion is less affected by feedstock variability than other process steps**. This result has significant positive implications for industry and should be validated with other organisms to assess general applicability. The modeling tool will enable rapid screening of new organisms on biomass-derived sugar and lignin substrates, enabling development of new biological pathways to create sustainable fuels and products.



Cross-cutting Analysis

OBJECTIVE: Quantify the industrially relevant economic and sustainability impacts of FCIC research and help guide future work using robust and well-documented techno-economic analysis (TEA) and life-cycle analysis (LCA) tools.

OUTCOME: The FCIC created and shared a dashboard of TEA and LCA case studies describing the economic and sustainability impacts of FCIC research.

IMPACT: Actionable insights that external stakeholders can use to help de-risk biorefinery design and operational decisions regarding feedstock variability.

Cross-cutting analysis work supported experimental research within the FCIC by quantifying the industrially relevant costs and environmental impacts of FCIC research. The interdisciplinary efforts leveraged well-documented and robust TEA and LCA modeling resources previously developed using BETO support⁹ to perform targeted analyses of specific research results to quantify how feedstock variability affects economic and sustainability metrics throughout the entire value chain, from feedstock production through preprocessing and conversion.

The results of these analyses were presented in TEA and LCA case studies focused on a specific process step or a group of process steps within the bioenergy value chain. The final milestone for the analysis work was to create and share a dashboard of TEA and LCA case studies describing the economic and sustainability impacts of FCIC research. This work was successful; the results of some of these focused case studies are shared in the Key Findings and Results section. A full list of these case studies is shared at the end of this report. In addition, FCIC researchers applied failure mode and effects analysis (FMEA) to identify and assess risks and potential mitigation strategies in selected conversion pathways.

⁹ National Renewable Energy Laboratory. 2024. "Bioenergy Models." Accessed Sep. 20, 2024. bioenergymodels.nrel.gov/models.



FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Techno-Economic Case Study:
Fermentation Cost Impacts from
Selected Critical Material Attributes



Cover page from the Oct. 2023 FCIC Techno-Economic Case Study, "Fermentation Cost Impacts from Selected Critical Material Attributes."



The FCIC Bioenergy Data Hub allows users to browse the results of FCIC research and download datasets of interest, fostering transparency and collaboration in the bioenergy community and maximizing the impact of FCIC research.

Data Integration

OBJECTIVE: Standardize how experimental data are organized and labeled, and provide a portal for public access to FCIC results, data, and software.

OUTCOME: FCIC researchers established the FCIC Bioenergy Data Hub, a publicly available repository that organizes and stores data and results produced by the FCIC, and developed an online community of industry stakeholders that uses the repository.

IMPACT: A publicly accessible repository that preserves FCIC research data, promotes broader collaboration between FCIC researchers and industry stakeholders, and enables these stakeholders to quickly leverage FCIC results for their applications.

Data integration work within the FCIC ensured that research results would be shared widely, a step that FCIC researchers recognize is a critical part of the mission. Publicly funded research must generate results that are “findable, accessible, interoperable, and reusable”—FAIR.¹⁰

The final milestone for this work was to establish a publicly available repository containing data and results produced by the FCIC and develop an online community of industry stakeholders using the repository. This work was successful: the FCIC Bioenergy Data Hub (hosted by the Pacific Northwest National Laboratory) is functional and has a group of industry stakeholders who have met in virtual FCIC-hosted meetings. FCIC researchers have contributed datasets from their research, and additional data and results from current and future BETO-sponsored industry projects will be added to serve as a resource to stakeholders in the future.

¹⁰ GO FAIR. 2024. “FAIR Principles.” Accessed July 9, 2024. www.go-fair.org/fair-principles/.



Strategies for Industry Impact

The FCIC used several strategies to maximize the impact of its work for bioenergy industry stakeholders. These strategies included:

- **Open-source models:** Releasing modeling codes as open-source to allow researchers and industry professionals to access, use, and build on FCIC research.
- **Publications:** Publishing scientific publications, technical reports, and conference presentations, with most of the scientific publications published in open-access formats to ensure wide availability to the scientific community, with the TEA/LCA reports released as publicly available case studies.
- **Data sharing:** Standardizing how experimental data are organized and labeled, and sharing these data publicly via the FCIC Bioenergy Data Hub.
- **Industry collaborations:** When possible, working directly with industry stakeholders on specific BETO-funded projects through CRADAs, which leverage FCIC capabilities, knowledge, and tools.

A New Paradigm for Critical Attributes—Beyond Composition, Moisture, Ash, and Particle Size

The traditional paradigm of feedstock variability considered feedstocks by name and routinely considered only a few properties—composition, moisture and ash content, and mean particle size. Although these properties are important, FCIC research has shown that each of these high-level properties actually represents categories of material attributes.

Biomass composition traditionally included the thermochemical measurements of ultimate and proximate analysis and the biochemical measurements of structural carbohydrates and lignin. Work in the FCIC expanded this category. FCIC researchers recognize substantial differences exist in these attributes among different anatomical fractions in biomass (e.g., corn cob vs. corn stalk, pine bark vs. pine white wood) and the ways these attributes respond to agronomic and process changes.

Moisture content considerations have moved beyond bulk moisture measurements to include the impacts of moisture on biomass attributes across the bioenergy value chain. These include moisture-induced degradation of biomass and moisture impacts on the physical and mechanical attributes that influence biomass handling and comminution. Expanding the understanding of how moisture impacts biomass degradation, handling, and comminution processes enables improved efficiency and reduced operational challenges across the bioenergy value chain.

Ash content measurements now recognize the importance of identifying and measuring the inorganic compounds comprising the ash fraction and whether these inorganics are an intrinsic part of the biomass itself or were introduced during harvest, storage, transport, or downstream processing. Different inorganic constituents can affect different parts of the biorefinery differently; impacts of specific inorganics on equipment wear and catalytic conversion processes are different. Although the intrinsic inorganic content is difficult to influence, preventing contamination by external inorganics is feasible. Detailed ash content analysis, including the identification of inorganic compounds, improves equipment longevity by reducing wear, enhances process efficiency, and will inform strategies to prevent contamination along the process chain.

Particle size considerations have expanded to include other physical and mechanical attributes such as PSD and particle shape, density, and porosity. In addition, mechanical attributes of biomass such as tensile, compressive, and shear strength and measures of toughness, hardness, and brittleness are critical material attributes. These and other physical and mechanical properties dictate biomass behavior in material handling and comminution processes.

Research in the FCIC has also reinforced that not all CMAs are equally important across all processes. For example, particle density is more important than particle porosity in physical processes such as material handling and comminution, whereas the opposite is true in chemical conversion processes, where intraparticle mass and heat transport phenomena in pores dominate. The expanded understanding of feedstock variability underscores its complexity, and the importance of taking a first-principles scientific approach to address it, across the entire bioenergy value chain.

Greater knowledge and transparency around biomass CMAs benefit all stakeholders across the bioenergy value chain—from feedstock suppliers to biorefinery operators. A more detailed understanding of biomass CMAs allows more precise valuation of the biomass resources and provides insight into how they are affected by harvest, transport, storage, and processing. The attribute differences among biomass anatomical fractions highlight potential opportunities in fractionating whole biomass streams, whereas the wide-ranging impacts of moisture emphasize the value in minimizing and monitoring the moisture content of biomass across the supply chain. Similarly, the impact of inorganics along the supply chain emphasizes the need to minimize and monitor possible contamination across the supply chain. The enhanced understanding of the importance of physical and mechanical attributes suggests that modifying equipment designs to accommodate a broader range of biomass feedstock types, such as purpose-grown crops, can be guided by fundamental measurements rather than relying on empiricism and heuristics.

This expanded knowledge empowers stakeholders to make smarter, data-driven decisions that optimize operations, mitigate risks, and maximize profitability, ultimately strengthening and de-risking the entire value chain.



Key Findings and Results

The detailed technical achievements of the FCIC are documented in more than 100 scientific publications, conference presentations, and technical reports, listed at the end of this report. Key findings and selected key results are highlighted here, again organized into three areas: biomass resource and feedstock characterization; biomass

handling, preprocessing, and wear analysis; and biomass conversion. The key findings are high-level lessons and observations from the detailed research performed in the FCIC, whereas the selected key results are illustrative of the breadth of work within the FCIC.



Biomass Resource and Feedstock Characterization



Biomass Handling, Preprocessing, and Wear Analysis



Biomass Conversion



Biomass Resource and Feedstock Characterization

Biomass resource and feedstock characterization work analyzed the biomass resources and feedstocks used by the FCIC to understand their intrinsic physical, chemical, and mechanical attributes and the ways these attributes are impacted by environmental, agronomic, and process-related factors. Researchers from the FCIC used advanced characterization tools to examine the structure and chemistry of biomass feedstock samples and worked closely with other FCIC researchers to understand how downstream processes are influenced by feedstock variability.

Key Findings

- There are large differences in the physical, chemical, and mechanical attributes of the anatomical fractions of herbaceous and woody biomass. Corn cobs are substantially different from corn stalks, and pine bark is substantially different from pine stem wood. These differences impact how these biomass materials perform in a biorefinery. A portion of the measured variability in bulk feedstock material attributes is driven by variations in the relative amounts of the individual anatomical fractions in individual samples. ***This knowledge will help biorefinery developers devise more tailored preprocessing and conversion strategies by accounting for the specific characteristics of the different anatomical fractions in their feedstock.***
- Moisture-induced degradation of biomass results in substantial changes to chemical, physical, and mechanical attributes. These changes can be monitored using advanced analytical techniques. The extent of these changes varies among the anatomical fractions. This suggests that ***targeted feedstock management strategies and careful tracking of biomass moisture content along the supply chain can provide more consistent feedstock supplies. Biomass degraded by exposure to moisture would likely have a lower value to end users but also may offer opportunities for biorefineries with conversion processes that can accept lower-quality material.***
- Drought-impacted corn stover showed minimal physical and chemical differences compared to nonstressed corn stover grown in the same location. Although further research could provide additional insights, the current findings ***suggest that drought conditions may not greatly affect the variability of corn stover attributes relevant for use as a feedstock for bioenergy production.***
- Solid waste streams such as MSW and landfill-bound MRF residues comprise different waste components (e.g., plastics, paper, cardboard, food waste), which have very different material attributes. Like biomass, the bulk properties of these waste streams are greatly influenced by the identity and relative amounts of these individual components. ***This knowledge allows biorefineries considering using waste feedstocks to consider more effective handling, sorting, and conversion strategies.***



Key Result: Characterizing Corn Stover

Agricultural residues such as corn stover are harvested seasonally, but biorefineries must operate year-round to be profitable. Improper storage of biomass feedstocks after harvesting can lead to unacceptable levels of degradation, dramatically decreasing the value of the feedstocks. Although the extent of degradation is typically measured as the loss in weight of individual bales—dry matter loss—the impact of degradation is much more complex. FCIC researchers used multiple advanced analytical tools to characterize the chemical and structural changes of corn stover.

Using an analytical technique called pyrolysis with multidimensional gas chromatography (py-GC/GC), researchers identified the breakdown products in corn stover samples with different biological degradation profiles, showing substantial fragmentation of the structural carbohydrates and more subtle changes in lignin components.¹¹

Other analytical techniques revealed significant lignin coalescence and condensation after degradation, along with changes in mechanical properties such as surface roughness and surface energy. Notably, the impact of degradation was not uniform across all corn stover anatomical fractions. The surface energy of the leaf fraction, which plays a role in wetting and interparticle adhesion, increased substantially after degradation, whereas the surface energy of both the cob and stalk fractions showed relatively little change. Not only does degradation alter fundamental biomass physical, chemical, and mechanical attributes but also the rate and manner in which these attributes change during degradation varies among fractions. These findings underscore the complexity of biomass feedstocks and emphasize the importance of precise, detailed characterization when studying biomass attribute changes. In addition, the findings reinforce the negative impact of biomass degradation beyond measures of dry matter loss

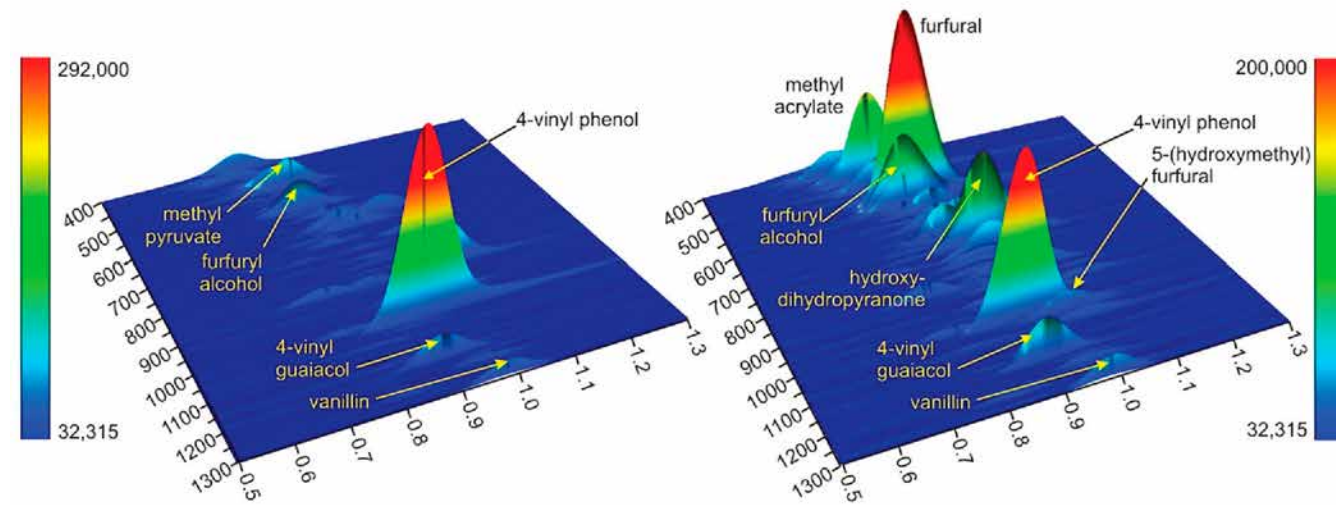


Figure 4. Detailed characterization of mildly degraded (left) and severely degraded (right) corn stover using pyrolysis with multidimensional gas chromatography (py-GC/GC) showed clear evidence of structural hemicellulose degradation.

¹¹ Groenewold, G. S., B. Hodges, A. N. Hoover, C. Li, C. A. Zarzana, K. Rigg, and A. E. Ray. 2020. "Signatures of Biologically Driven Hemicellulose Modification Quantified by Analytical Pyrolysis Coupled with Multidimensional Gas Chromatography Mass Spectrometry." *ACS Sustainable Chemistry & Engineering* 8 (4). [10.1021/acssuschemeng.9b06524](https://doi.org/10.1021/acssuschemeng.9b06524).

and the importance of minimizing degradation through proper storage and transport—keeping the biomass as dry as possible for as long as possible.¹²

In another study, FCIC researchers compared corn stover harvested during a drought year to corn stover from the same location but from a year receiving normal rainfall. Surprisingly, the drought-stressed corn stover showed minimal physical and chemical differences compared to the nonstressed corn stover. Although overall harvest yield (the amount produced per acre) was dramatically reduced in the drought year, the harvested stover was surprisingly similar in properties. This suggests that, although drought will dramatically reduce the total quantity of stover available in a given area, the composition and convertibility of the stover are nearly identical to that during a nondrought year.

¹² Feedstock Variability: Causes, Consequences and Mitigation of Biological Degradation, *Biomass Magazine* (2023) - <https://biomassmagazine.com/articles/feedstock-variability-causes-consequences-and-mitigation-of-biological-degradation-19639>.

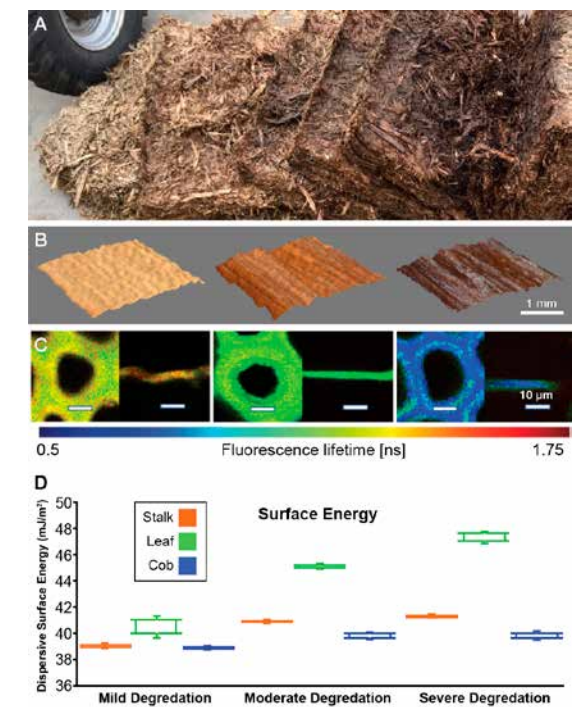


Figure 5. Advanced analytical tools used to examine a visibly degraded corn stover bale (A) showed substantial differences among mild, moderate, and severe degradation in multiple attributes including (B) surface roughness, (C) lignin chemistry as measured by fluorescence lifetime, and (D) surface energy of multiple anatomical fractions.



Biomass Handling, Preprocessing, and Wear Analysis

Biorefineries are complex systems with multiple process steps that convert biomass resources into valuable and sustainable fuels and chemicals. In addition to the chemical conversion steps (discussed later), steps upstream in the process play a vital role. These steps include material handling—moving the biomass on conveyor belts or into and out of bins and hoppers, and comminution—decreasing the size of the biomass. The variability of biomass resources can affect both the material handling and the comminution steps by causing inconsistent operations and process interruptions. In addition, the equipment used in these steps may experience wear during operation, leading to poor performance and unexpected interruptions.

Key Findings

- Empirical approaches to predict material handling and comminution performance have been unsuccessful. A combined experimental and computational approach to understanding biomass flow and comminution behavior was shown to be effective. ***This approach has provided better insights into how biomass behaves in material handling and comminution processes and will inform improved equipment design and operation.***
- Separating biomass into its anatomical fractions during preprocessing adds nominal cost to the overall process but can provide substantial flexibility in designing, operating, and optimizing downstream conversion operations, for example by converting the fractions separately or diverting a particular fraction to another use. ***This downstream flexibility could translate to improved overall system economics and increased process reliability.***
- Moisture management during preprocessing can reduce costs and save energy. For example, milling higher moisture biomass prior to drying decreases throughput and increases mill energy usage, leading to higher milling costs. However, removing off-specification material after milling but before drying can reduce dryer energy use enough to result in reduced overall costs¹³ and lower energy use.¹⁴ ***Optimizing moisture management in preprocessing operations can result in significant savings in energy and operational costs and improve process efficiency, reliability, and sustainability in comminution and drying operations.***
- Wear in biomass processing equipment is driven by three factors—the identity and concentration of the inorganic components in the biomass (commonly called ash), the mechanical design of the equipment, and the materials of construction of the equipment. ***Understanding how these key factors interact is necessary to develop effective wear mitigation strategies.***
- Mitigating equipment wear by modifying biomass processing equipment (e.g., changing the materials of construction or redesigning key parts) is a cost-effective strategy to minimize maintenance costs and avoid unplanned process interruptions. ***Wear mitigation improves process performance and reliability and leads to significant long-term savings and greater profitability.***
- Inorganic materials in biomass, both those naturally present and those accidentally introduced during harvest, transport, and storage, cause equipment wear and reduce biomass feedstock quality. ***Preventing the introduction of or removing added inorganic materials early in the overall process will substantially improve feedstock quality, process reliability, and profitability.***

¹³ FCIC Case Study - Impact of moisture and grinder type on throughput and energy consumption of comminution of anatomically fractionated corn stover. In publication process.

¹⁴ FCIC Case Study - Life-Cycle Greenhouse Gas Emission Impacts of Forest Residue Pre-processing with Wet Milling (2023). <https://www.osti.gov/biblio/1994908>.



Key Result: Improving Biomass Material Flow

The movement of biomass materials through a biorefinery—on weigh belts, on feed conveyers, and into and out of bins and hoppers—has long been a critical problem for biorefinery scale-up. Empirical approaches to adapt bulk material handling equipment from other industries have failed largely because biomass materials are fundamentally different from other bulk materials having more regular particle shapes and sizes, such as powders and grains.

FCIC researchers have worked to address this problem—understanding and then predicting the flow behavior of heterogeneous bulk solids under different conditions—starting with the first-principles scientific fundamentals to understand the physics of biomass conveyance and then using a combination of careful experimental measurement techniques and physics-based computational modeling to develop knowledge and tools to help industry stakeholders design functional systems.

Using a wide variety of conventional laboratory-scale instruments, FCIC researchers measured the physical and mechanical properties of various biomass feedstocks under both static and dynamic conditions.¹⁵ These studies provided valuable data and insights into how biomass feedstocks behave under different conditions. Additionally, they used novel, larger-scale systems for pilot-scale measurements of bulk flow characteristics,¹⁶ generating useful data that connect the mechanical and physical properties of biomass particles to their bulk-scale material flow behavior.

At the same time, FCIC researchers developed and validated a collection of computational models to describe and predict the bulk flow of biomass under a range of conditions. These models use different physics-based approaches (e.g., continuum vs. discrete element modeling [DEM]) and vary in complexity and computational intensity. Detailed descriptions of these modeling tools have been



Figure 6. A variety of laboratory- and pilot-scale characterization tools were used to measure the physical and mechanical properties of biomass feedstocks under both static and dynamic conditions and to validate computational models of biomass flow. From left to right: Laboratory-scale rheometer, laboratory-scale uniaxial compression cell, pilot-scale adjustable wedge hopper discharge, and pilot-scale inclined plane flow tester.

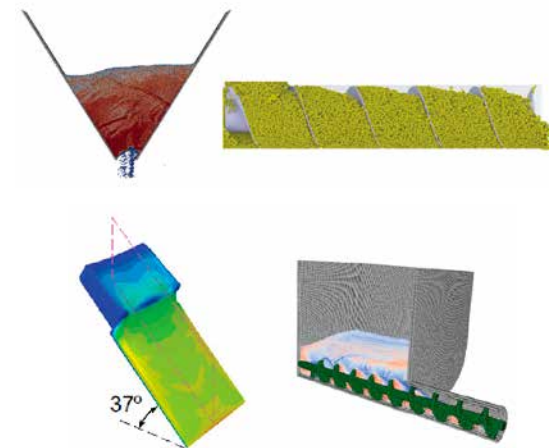


Figure 7. A collection of computational models that describe and predict the bulk flow of biomass, using different physics-based approaches and varying in complexity, provide useful tools for industry stakeholders. (L-R) Wedge hopper, auger, inclined plan flow tester, hopper/auger combination.

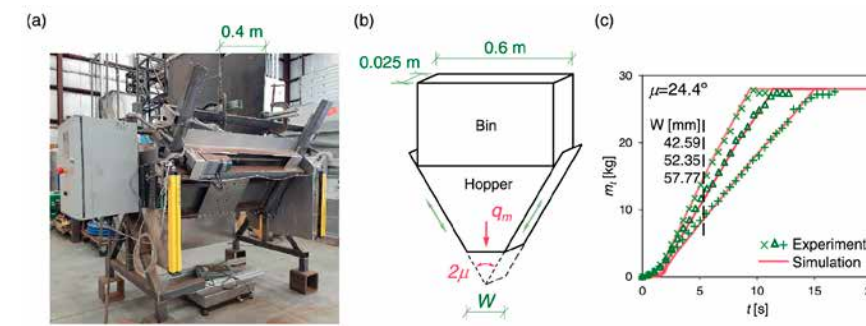


Figure 8. (A) An adjustable wedge hopper collects experimental data on different hopper angles and outlet widths. (B) A physics-based computational model is developed and validated with additional experimental data (C), making it a useful tool for simulating wedge hoppers of various sizes.

published in many peer-reviewed articles, and computer codes are available as open-source software packages (see Open-Source Modeling Tools for descriptions of and links to these tools).

FCIC researchers provided a practical demonstration of how these modeling tools can be applied.¹⁷ They first developed and validated a computational model of pine residue flow in wedge-shaped hoppers, using experimental data from a wedge hopper with adjustable hopper inclination angles and outlet widths. Once the model was validated with additional experimental data, it became a tool for simulating biomass flow in wedge hoppers of different dimensions.

By running numerous simulations with different values of two hopper design parameters—wall friction and inclination angles—and different values of a parameter to characterize the biomass material called internal friction angle, FCIC researchers generated detailed velocity profiles for different combinations of these parameters. To make these results more accessible, they simplified these velocity profiles to a single term, the mass flow index, a measure of flowability. A design chart for a specific biomass material can then be generated for different wedge hopper configurations by selecting simulations from this large dataset based on specific values of the biomass parameter.

Although the bulk flow of bulk biomass materials remains a complex issue, the FCIC has established a robust modeling and experimental framework

to characterize the flow performance and bulk properties of biomass materials at different scales. The FCIC has also generated a wide range of experimental datasets to calibrate and test even more advanced flow models as they become available.

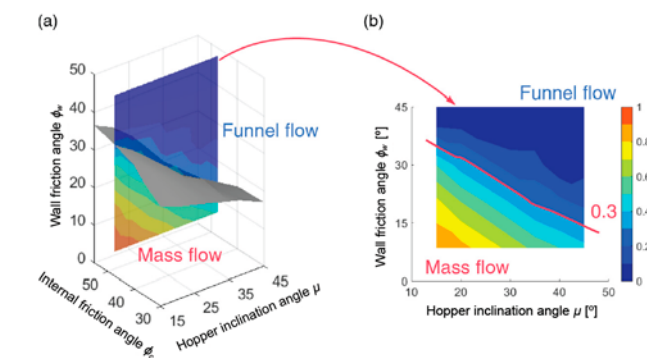


Figure 9. The wedge hopper design tool helps analyze how material attributes and process parameters affect hopper performance. (A) Simulations with different values of wall friction, internal friction, and hopper angle produce various flow patterns, simplified to a mass flow index. Mass flow index values below 0.3 indicate desirable “mass flow” conditions, while values above 0.3 show undesirable “funnel flow” conditions. (B) A design chart for pine residues shows that lower hopper angles and wall friction values lead to desirable mass flow.

¹⁵ Effect of Moisture and Feedstock Variability on the Rheological Behavior of Corn Stover Particles. *Frontiers in Energy Research*. (2022). <https://doi.org/10.3389/fenrg.2022.868050>.

¹⁶ Multiscale Shear Properties and Flow Performance of Milled Woody Biomass. *Frontiers in Energy Research* (2022). <https://doi.org/10.3389/fenrg.2022.855289>.

¹⁷ Wedge-Shaped Hopper Design for Milled Woody Biomass Flow. *ACS Sustainable Chemistry & Engineering* (2022). <https://doi.org/10.1021/acssuschemeng.2c05284>.



Key Result: Predicting Biomass Comminution Performance

Preprocessing refers to the operations and treatments applied to biomass resources to make them suitable for further processing or conversion. This area of research within the FCIC focused on understanding the fundamentals of comminution of biomass materials, a critical step in preprocessing, to develop experimentally validated tools and knowledge to predict how biomass properties affect different comminution unit operations.

FCIC researchers have taken multiple approaches to model the behavior of comminution equipment. One approach is population balance modeling, a statistical method that predicts the PSD of knife-milled biomass based on a limited set of experimental measurements.¹⁸ Even more computationally intense, the DEM for knife milling combines a detailed model of the knife mill along with biomass physical and mechanical properties to predict large-scale comminution performance.¹⁹

Researchers from the FCIC also used molecular modeling techniques to predict rather than measure biomass mechanical properties. The team developed the first experimentally derived atomistic model for a plant cell wall reported in the literature, and the first to be placed in a public archive. Through molecular dynamics simulations using this model, they quantified the contributions of each biopolymer constituent to the mechanical properties of biomass tissue.²⁰ This work enables the prediction of mechanical properties of lignocellulose assemblies as a function of biopolymer composition and macromolecular architecture. It has already been successfully used by an industry partner to understand how biopolymer additives affected the mechanical properties of cellophane and other cellulose composites and to suggest novel formulations to further improve material performance.

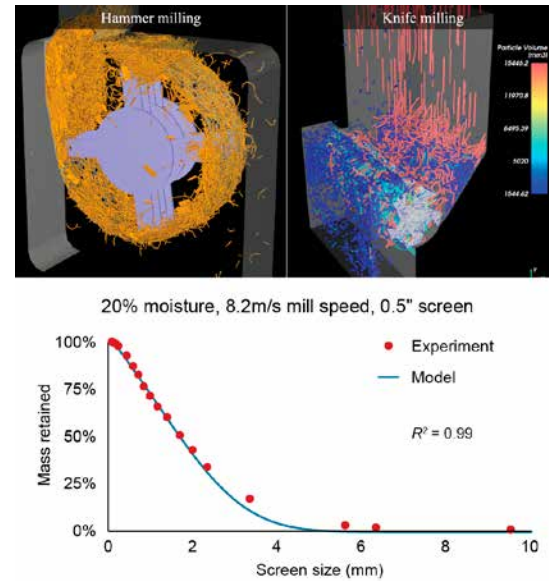


Figure 10. Experimentally validated computational models describing and predicting the comminution behavior of biomass provide useful tools for industry stakeholders.

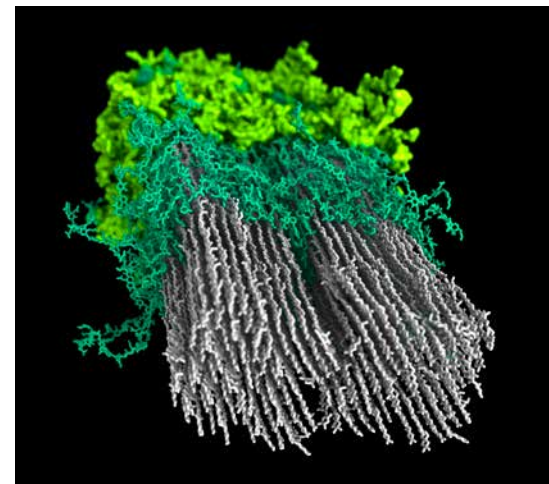


Figure 11. Depiction of a macromolecular model for the lignocellulose assembly in poplar wood secondary cell walls. Cellulose is shown in white, hemicellulose in dark green, and lignin in light green.

¹⁸ Predicting biomass comminution: Physical experiment, population balance model, and deep learning. Powder Technology (2024). <https://doi.org/10.1016/j.powtec.2024.119830>.

¹⁹ An experiment-informed DEM study of knife milling for flexural biomass feedstocks. Biosystems Engineering (2023). <https://doi.org/10.1016/j.biosystemseng.2023.10.008>.

²⁰ Atomistic, macromolecular model of the populus secondary cell wall quantitatively informed by solid-state NMR. Science Advances (2024). <https://doi.org/10.1126/sciadv.adi7965>.



Key Result: Understanding and Mitigating Equipment Wear

FCIC researchers addressed an important but often overlooked risk associated with scaling up biorefineries—wear-induced failures of biomass processing equipment. Biomass processing equipment often experiences significant wear because of the presence of inorganic materials in biomass, causing equipment downtime and process interruptions.

The mechanisms behind equipment wear are complex and influenced by several factors: the characteristics of the biomass being processed, the properties of the materials used to make the processing equipment, the equipment design, and the equipment operating conditions. For example, different types of biomass comminution equipment, although performing the same function of reducing particle size, can have very different wear modes. Knife mills and hammer mills, which operate at relatively high rotational velocities, typically

experience erosive wear, whereas shredders and rotary shear equipment, which operate at lower rotational velocities, typically experience abrasive wear. Because these wear modes are different, potential mitigation approaches are different.

Researchers from the FCIC with decades of experience in the science of wear—called tribology—demonstrated the first step in mitigating wear is to accurately identify the precise type of wear, the construction materials of the equipment, and the wear-inducing species in the biomass. Only after this analysis should mitigation options be considered, tested, and then selected.

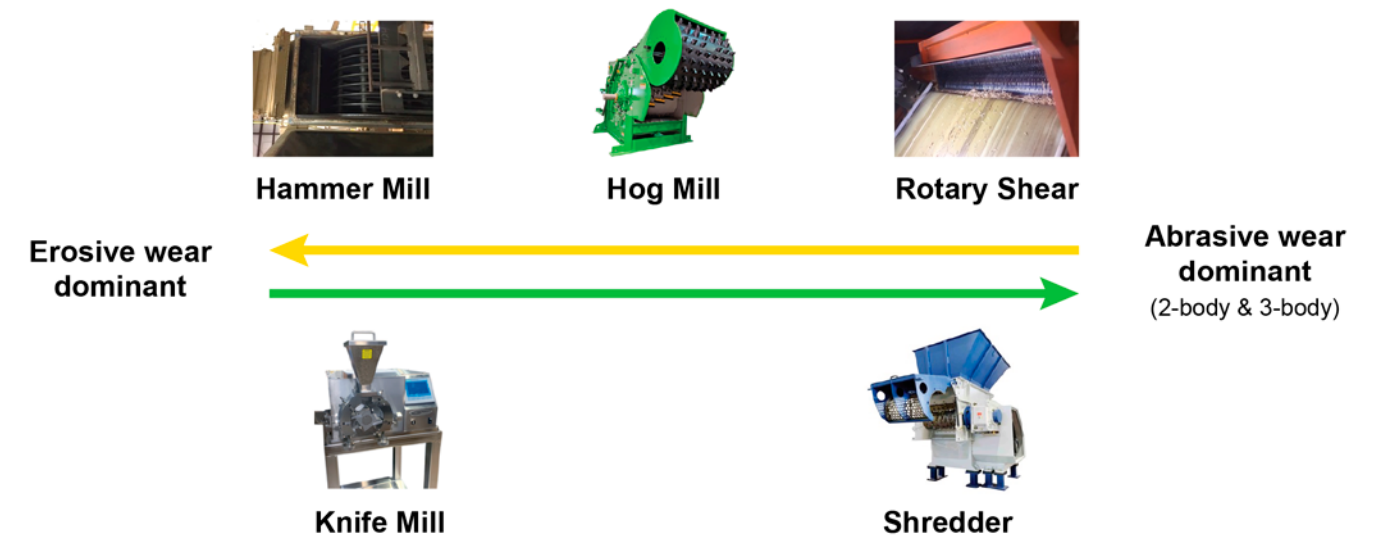


Figure 12. Understanding the mechanism causing equipment wear is the first step in identifying mitigation approaches. Different types of comminution equipment used in the bioenergy industry sector have very different operating principles which in turn mean they can have very different wear mechanisms.



Addressing wear issues can reduce processing costs and improve plant operations. In a study^{21,22} on corn stover comminution using a knife mill, the team showed the additional costs incurred by either using wear-resistant materials or applying wear-resistant coatings to existing materials resulted in substantial savings. The longer-lasting milling equipment not only reduced equipment maintenance costs but, more importantly, decreased the frequency of process interruptions. This led to extremely short payback periods and internal rates of return exceeding 1000%, highlighting the clear financial benefits of investing in wear-resistant solutions.

By combining deep subject matter expertise, advanced characterization, and modeling techniques, FCIC researchers produced multiple scientific publications and presentations, two collaborative projects with industry partners, and a recent contribution for more general audiences summarizing the overall approach.²³ Clearly, wear is a ubiquitous phenomenon in biorefineries, and FCIC research has shown the value of pursuing science-based wear mitigation strategies across an entire facility.

²¹ Improving knife milling performance for biomass preprocessing by using advanced blade materials. *Wear* 522(2023). <https://doi.org/10.1016/j.wear.2023.204714>,
²² FCIC Case Study – Value Proposition of Coatings or New Alloys on Hammer Wear. (2023). <https://www.osti.gov/biblio/1994909>.
²³ “Developing Science-Based Tools and Solutions to Enhance Reliability and Efficiency of Biomass Preprocessing”, *ASABE Resource Magazine* (accepted, in press)



Key Result: Failure Mode and Effects Analysis of Feedstock Production

FMEA is a systematic criticality assessment tool that combines subject matter expertise with the QbD framework to provide semiquantitative evaluations of failure risk in manufacturing processes. This method assesses risks by examining the severity, occurrence, and detectability of specific process deviations. For example, a frequently occurring deviation with severe consequences that is difficult to detect would result in a very high risk, whereas a rare, easily detected deviation with minimal impact would represent a very low risk.

FCIC researchers applied the FMEA approach to both the high- and low-temperature conversion pathways, focusing on risks associated with producing acceptable feedstocks for conversion—pine residue for pyrolysis and corn stover for DMR/EH followed by microbial conversion.²⁴ The FMEA targeted failures related to meeting CMA for

each pathway’s conversion steps. They identified deviations in moisture and fixed carbon content as the most critical risks for the high-temperature pathway and deviations in particle size and both carbohydrate and ash content as the most critical risks in the low-temperature pathway.

The application of FMEA offers process developers actionable insights to prioritize and mitigate specific risks in biomass conversion. Using a targeted risk reduction approach such as FMEA enables developers to optimize feedstock quality, reduce operational risks, enhance process reliability, and lower costs associated with process failures, contributing to more sustainable and scalable bioenergy production.

²⁴ Failure Mode and Effects Analysis Summary Report (July 2023). <https://www.osti.gov/servlets/purl/1994910>.





Biomass Conversion

Like other parts of the bioenergy value chain, a key scale-up risk for biorefinery conversion operations is the challenge of predicting the impact of variable feedstock properties on the performance of a larger reactor using performance data from smaller systems. Because the conversion reactor is typically a very expensive component of biorefineries, minimizing reactor performance risk is critical to de-risking the scale-up process. The primary objective of this work was to develop a science-based understanding of how variations in feedstock attributes affect conversion performance in both low- and high-temperature pathways. This deeper understanding will help address the inherent variability in biomass feedstocks and the influence of operational conditions on the final product.

The goals included developing two experimentally validated frameworks: (1) a multiscale computational framework for predicting high-temperature conversion performance and (2) an artificial intelligence/machine learning framework for predicting microbial conversion performance of cellulosic sugar and soluble lignin streams in the low-temperature pathway. Both frameworks will enable biorefineries and industry operators to design conversion processes that are flexible and responsive to feedstock variability, allowing them to proactively manage feedstock quality and process conditions for more stable and efficient operation of conversion reactors.

Key Findings

- The microbial conversion of biomass-derived sugar and lignin streams is influenced primarily by process variability rather than by differences in the feedstock composition. Although different biomass types and deconstruction methods yield sugar and lignin streams of different composition, the conversion rates, titers, and yields of these streams in microbial conversion were similar. Thus, although more work is needed, **the risk of microbial conversion performance variability resulting from differences in feedstock composition appears minimal.**
- Different anatomical fractions of corn stover showed substantial differences in pretreatment yields via DMR/EH to produce soluble sugars and lignin.²⁵ This suggests **optimizing the conversion performance of the individual fractions separately can increase overall process yields, although at the expense of increased operational complexity.**
- Corn stover impacted by drought showed no measurable differences in DMR/EH conversion yields compared to nonstressed corn stover. Although the drought dramatically decreased overall harvest yield, the critical material attributes of the stover associated with low-temperature conversion were essentially unchanged, suggesting that, **although the feedstock supply risks associated with drought include substantially reduced harvest yield, they do not include reduced conversion performance, mitigating concerns about feedstock quality during droughts.**
- Measured differences in fast pyrolysis conversion yields of pine residues from forest thinnings and timber harvests were largely the result of differences in the relative amounts of their anatomical fractions. **Recognizing the importance of the constituent anatomical fractions provides process developers additional flexibility in designing both pyrolysis reactors and feedstock handling systems upstream to improve process reliability and overall profitability.**

²⁵ FCIC Case Study – Techno-Economic Case Study: Low Temperature Performance Based on Isolated Anatomical Fractions of Corn Stover. <https://www.osti.gov/servlets/purl/1996903>.



Key Result: A Multiscale Thermochemical Modeling Framework

Predicting the effects of variable feedstock material attributes and reactor process parameters on the performance of thermochemical reactors for gasification and fast pyrolysis is difficult because there are important phenomena occurring simultaneously at very different length scales.

At the molecular scale, biomass feedstocks undergo a very complex set of chemical reactions to produce the desired products (bio-oil for fast pyrolysis and synthesis gas for gasification) along with solid biochar and light gases. Understanding the intrinsic kinetics of these reactions is critical. However, at the particle scale, the chemical composition limits the overall yield, and individual feedstock particle size, morphology, and porosity affect the speed of the molecular-scale reactions. Heat must diffuse into the particles, and reaction products must diffuse out. Finally, at the reactor scale, the reactor shape and size, along with its operating conditions, affect the temperatures the biomass particles are exposed to and the duration of this exposure.

FCIC researchers first used careful laboratory experiments to generate robust, reproducible primary data on the conversion of well-characterized biomass materials and then detailed physics-based particle-scale modeling to extract kinetic parameters to populate well-accepted theoretical reaction schemes. These particle-scale models relate feedstock attributes such as particle size and shape distributions, composition, moisture content, and thermal properties to thermochemical conversion behavior. These particle-scale models are too computationally intensive to implement at large scale and must be simplified before they can be used in reactor-scale computational fluid dynamics (CFD) models. These simplified models are incorporated into the reactor-scale simulations via machine-learned correlations, enabling pilot- and industrial-scale models to accurately account for feedstock-specific kinetic effects while also capturing reactor-scale dynamics.^{26,27}

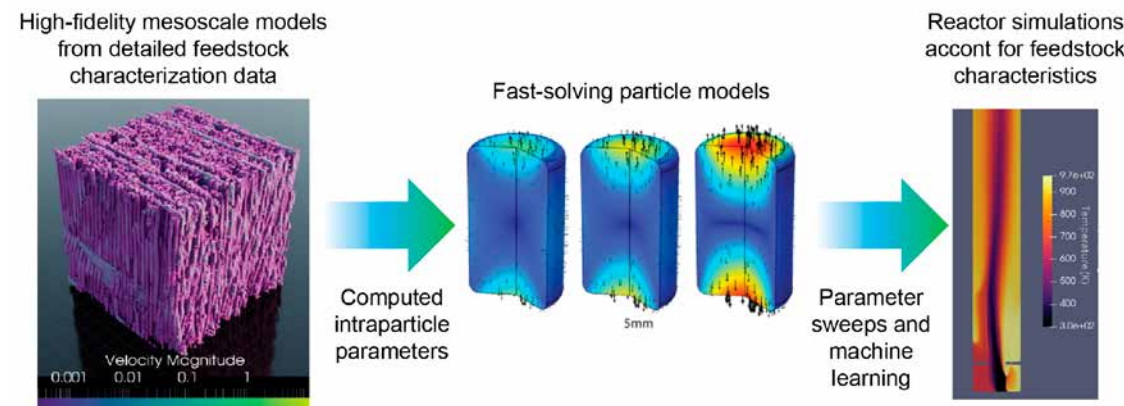


Figure 13. Schematic depiction of multiscale modeling. (Left) Simulation of fluid flow through the microstructure of Douglas fir wood obtained by x-ray computed tomography. (Center) Particle models with anisotropic transport properties determined from microstructure simulations are used to predict how variations in feedstock attributes impact product yields and required conversion times. (Right) Parametric sensitivity analysis combined with machine learning allows reactor models to account for detailed feedstock-specific effects.

²⁶ Advances in multiscale modeling of lignocellulosic biomass. ACS Sustainable Chemistry & Engineering (2021). <https://doi.org/10.1021/acssuschemeng.9b07415>.

²⁷ Multiscale CFD simulation of biomass fast pyrolysis with a machine learning derived intra-particle model and detailed pyrolysis kinetics. Chemical Engineering Journal (2021). <https://doi.org/10.1016/j.cej.2021.133853>.

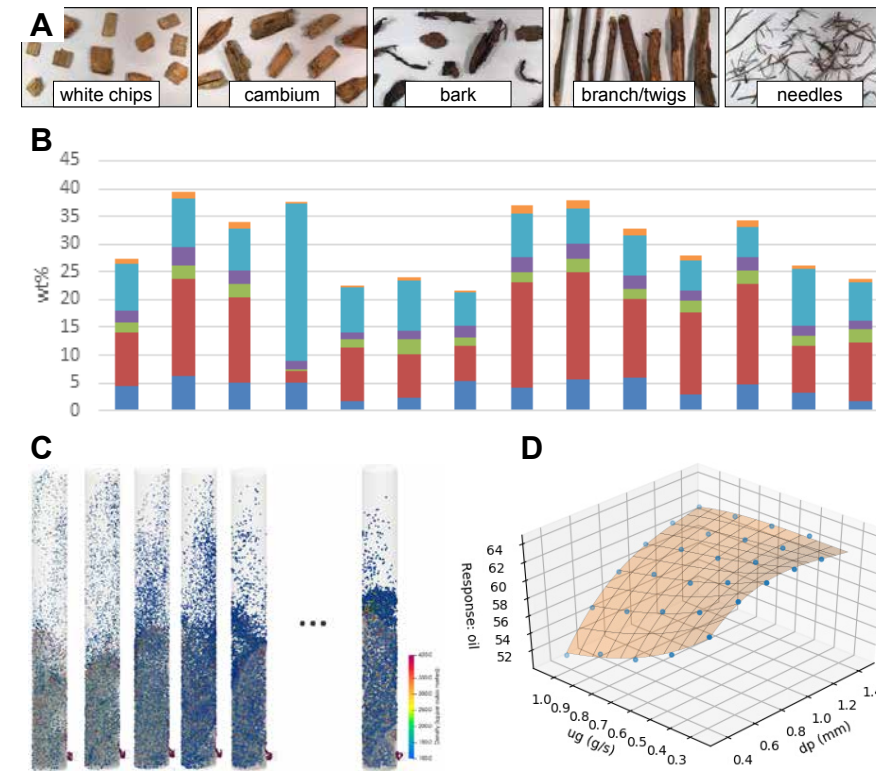


Figure 14. Careful (A) biomass characterization and (B) experimental data generated in laboratory-scale systems provide conversion data that can be combined with structure and morphology information to extract intrinsic kinetics. (C) These kinetic models are then simplified and used in reactor-scale CFD models of thermochemical conversion reactors to perform parametric sensitivity analyses and (D) generate reactor operational maps such as pyrolysis oil yield as a function of feed rate and mean particle size.

Once validated by careful laboratory work, these integrated modeling frameworks are also valuable for TEA and LCA studies. They can estimate reactor performance (e.g., product yields) in large-scale reactors over ranges of feedstock attributes and reactor process parameters. Systematically varying the inputs to these computationally intensive models facilitates creation of a map of reactor yields. These yield maps can be used to create much simpler “reduced-order” models relating feedstock and reactor properties to reactor performance for use in TEA and LCA studies.

In one example, FCIC researchers recently used the pyrolysis modeling framework to study the impact of air classification techniques on fast pyrolysis performance.²⁸ The team performed air classification experiments on pine residues, systematically varying the moisture content and air classification conditions to generate a collection of fractionated residues. They characterized these

residues and used these data and the pyrolysis modeling framework to perform “virtual” conversion experiments on these fractionated residues, saving substantial time and money compared to conventional laboratory pyrolysis experiments.

In another example, FCIC researchers used the pyrolysis modeling framework to understand the impacts of feedstock attribute variability on process economic variability,²⁹ showing for one scenario that the variability in overall process economics was driven by inorganic content and extractives content of pine residues. In other work, FCIC researchers used the modeling framework to study the overall process economics of pine thinnings and pine harvest residues, showing that the two residue types provided similar overall process economics because of similar conversion yields and feedstock supply costs.³⁰

²⁸ The effect of air separations on fast pyrolysis products for forest residue feedstocks. Fuel (2024). <https://doi.org/10.1016/j.fuel.2024.132572>.

²⁹ A simplified integrated framework for predicting the economic impacts of feedstock variations in a catalytic fast pyrolysis conversion process. Biofuels, Bioproducts & Biorefining (2021). <https://doi.org/10.1002/bbb.2319>.

³⁰ FCIC Case Study - Comparative Techno-Economic Analysis of Available Feedstocks for High-Temperature Conversion: Whole Tree Thinnings and Mature Pine Residues (2023). <https://www.osti.gov/biblio/1996902>.



Key Result: Predicting Microbial Conversion Performance

The vast range of possible deconstruction chemistries, potential biocatalysts, and products makes it challenging to predict the effects of variable feedstock composition and process parameters on the performance of low-temperature biomass conversion processes that use different deconstruction chemistries to produce convertible sugar and lignin streams, as well as different biocatalysts to upgrade these streams.

FCIC researchers used a combined experimental and modeling approach to address this challenge. First, the researchers used a standard deconstruction chemistry—DMR/EH—to produce convertible sugar and soluble lignin streams from multiple corn stover materials, which then underwent separate biocatalytic transformations (sugar streams to 2,4-butanediol, butyric acid, or bisabolene, and lignin streams to muconic acid). By using careful experimental design approaches and performing detailed chemical characterization, they generated a robust dataset of conversion performance variability on different corn stover

samples, including individual anatomical fractions and drought-impacted materials. There were measurable differences in the DMR/EH results among the anatomical fractions, which in turn led to differences in the overall process economics.³¹

Careful analysis of the dataset using a variety of statistical tools and substantial subject matter expertise revealed multiple critical material attributes—characteristics of the feedstock and conversion process that substantially affect performance. The researchers expected that many of the most critical attributes would be related to the corn stover samples themselves—how they were grown, harvested, and stored. Surprisingly, the most impactful variables are process related. For the samples explored within the FCIC, the impacts of intrinsic feedstock variability were substantially smaller than differences among conversion process variability,³² suggesting that the perceived risk of feedstock variability on biorefineries can be substantially reduced upstream of the microbial conversion step. Thus, the risk of microbial

conversion performance variability resulting from differences in feedstock composition appears minimal, and additional research to mitigate the negative impacts of feedstock variability may best be directed upstream of the microbial conversion step.

Equally important to the experimental work, FCIC researchers used machine learning approaches to integrate the experimental data with biocatalytic profiles generated from libraries of biocatalysts. This ensured the experimental results are broadly applicable to other biocatalyst/biointermediate systems. The researchers also provided insights into the potential microbial conversion performance of other biocatalysts, allowing industry stakeholders to rapidly screen libraries of potential biocatalysts for microbial conversion performance to identify potential candidates for more detailed research and development.

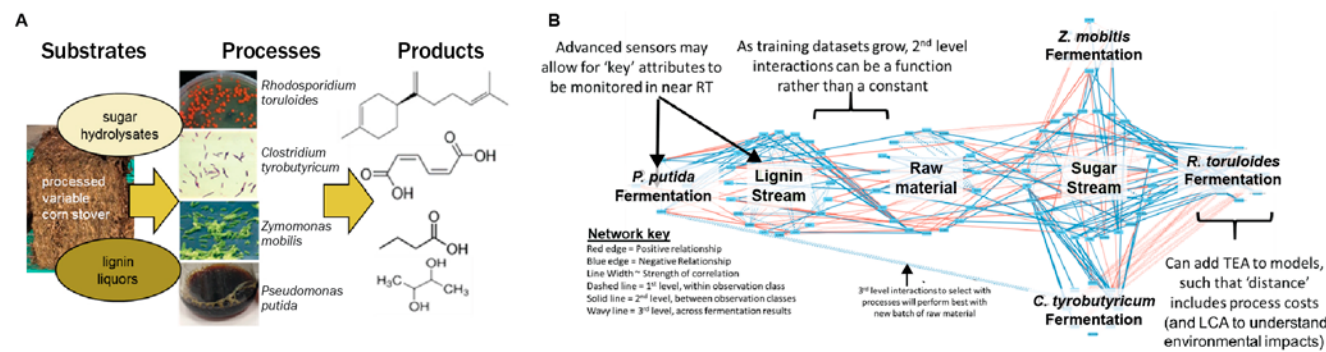


Figure 15. (A) Understanding the impact of feedstock variability on the microbial conversion performance of both sugar and lignin streams produced from corn stover by multiple biocatalysts requires detailed characterization of feedstocks and intermediate streams along with careful experimental approaches to understand the rates of biocatalyst growth and bioproduct formation from these intermediate streams. (B) By combining these data with metabolic modeling aided by machine learning approaches, it is possible to generalize these results to reliably predict the performance of other biocatalysts and other biomass feedstocks.

³¹ FCIC Case Study: Low-Temperature Conversion Performance Based on Isolated Anatomical Fractions of Corn Stover. DOE/EE-2692 (July 2023). <https://www.osti.gov/biblio/1992831/>.

³² Feedstock variability impacts the bioconversion of sugar and lignin streams derived from corn stover by *Clostridium tyrobutyricum* and engineered *Pseudomonas putida*. Microbial Biotechnology (2024). <https://doi.org/10.1111/1751-7915.70006>.

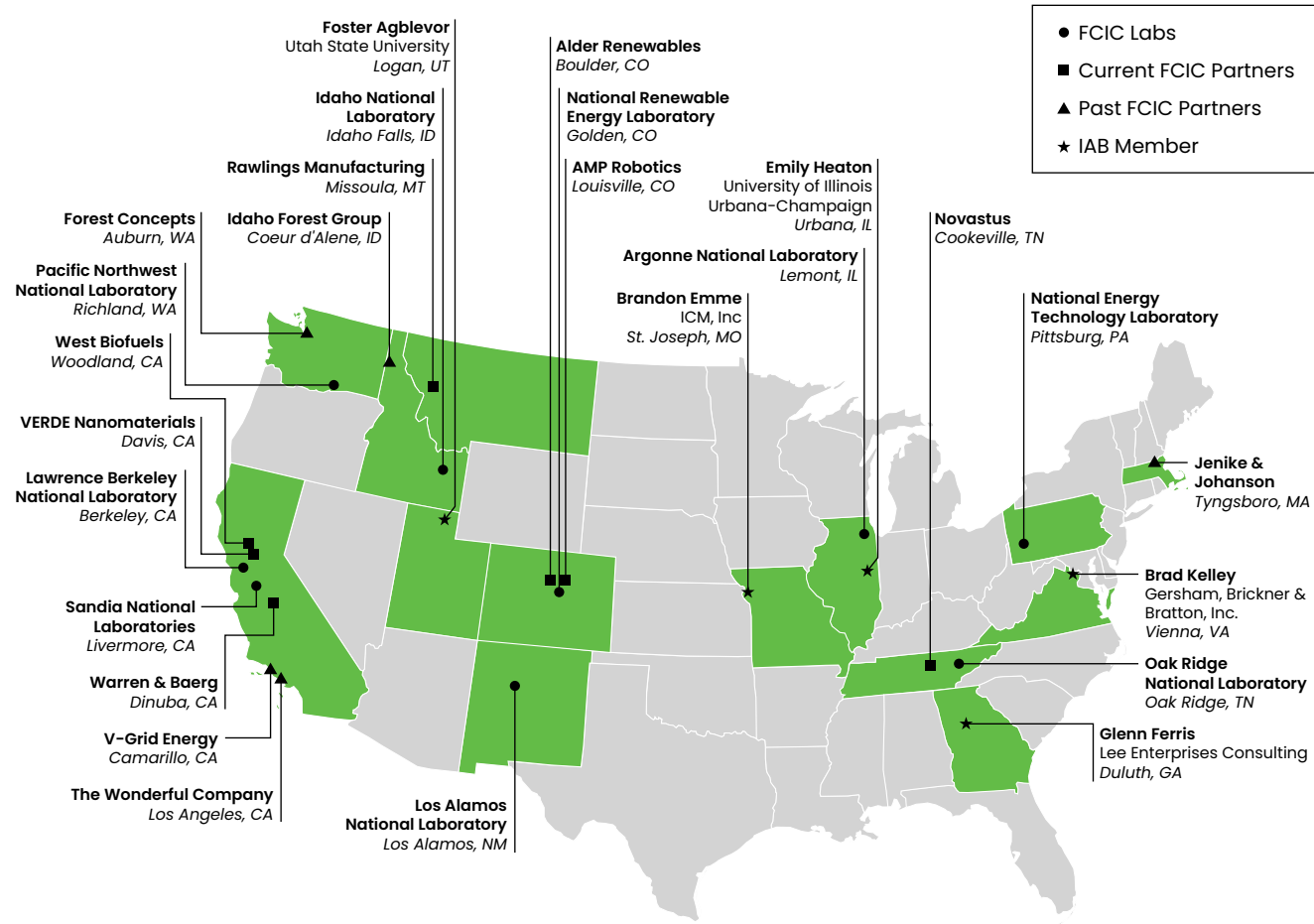


In the Future

In the future, FCIC researchers will continue to understand, measure, and mitigate the impacts of feedstock variability across the bioenergy/bioproducts value chain. However, the focus will be on directly supporting industry stakeholders by deploying the knowledge and tools developed in collaborative but industry-led projects, similar to the successful CRADA calls the FCIC has performed in the past.

The FCIC will continue to remain a resource to industry stakeholders, adding information to the FCIC website at <https://energy.gov/fcic>, capturing the results of future projects, and continuing outreach activities to industry to ensure FCIC work is shared widely. The FCIC will also continue to add additional datasets to the FCIC Bioenergy Data Hub and update publications, including scientific publications, TEA/LCA case studies, and conference presentations. Through these efforts, the FCIC will ensure results that continue to de-risk the scale-up of biorefinery technologies.

Partners and Stakeholders



Map of FCIC partner national laboratories, CRADA call recipients, and Industry Advisory Board members.

BETO Program Representatives

Mark Elless
Technology Manager, Renewable Carbon Resources

Beau Hoffman
Technology Manager, Conversion Technologies

Ben Simon
Technology Manager, Systems Development and Integration

Valerie Sarisky-Reed
Director, Bioenergy Technologies Office

Industry Advisory Board

The FCIC has benefited greatly from the insight and feedback from our Industry Advisory Board. Through regular virtual meetings and frequent informal conversations, they have generously provided their wisdom and guidance to help FCIC researchers focus their efforts and understand the current and future challenges of the bioeconomy.

Foster Agblevor, Professor, Utah State University

Brandon Emme, Director of Technology Development, ICM

Glenn Ferris, Managing Director, Lee Enterprises

Emily Heaton, Professor, University of Illinois

Brad Kelley, Senior Project Engineer; Gershman, Brickner & Bratton



Consortium Impacts

The project successfully executed all the planned impact strategies. This included the release of open-source modeling tools, the publication of research findings in open-access journals, the establishment of a public data repository, and the execution of several industry-led research projects.

Open-Source Modeling Tools

FCIC researchers have developed several open-source software tools that can be used by industry and academic stakeholders to understand and optimize biomass preprocessing and conversion processes. These tools enable users to model and predict how different biomass materials will perform during various stages of the bioenergy value chain, from handling and comminution to chemical transformation. By leveraging these models, stakeholders can advance the scientific development of biomass conversion technologies.

ABRADE—an open-source MS Excel-based model for predicting edge recession rate in knife mill cutters caused by abrasion by inorganic particles entrained in biomass feedstock. This tool can be used by industry stakeholders to predict the rate that knife mill blades will wear down during use (a phenomenon called “edge recession”) from knowledge of the knife mill and feedstock properties. The tool can be used to forecast how different blade materials will affect blade lifetimes, allowing them to balance the costs and benefits of the different materials.

<https://www.anl.gov/amd/abrade-model>

Granular Flow Models—a collection of open-source subroutines for modeling granular flow physics in the popular flow modeling software Abaqus™ allows users to predict the flow behavior of complex granular materials such as milled biomass. This enables equipment designers to better understand biomass flow in equipment such as hoppers and bins. <https://github.com/idaholab/GranularFlowModels>

BDEM/Exagoop— BDEM, or Biomass Discrete Element Method, is a simulation tool used to model granular flows, particularly for biomass materials. Exagoop is a related tool that focuses on simulating multiphase problems. These tools allow users to simulate complex material behaviors and can be used to simulate biomass flows in different geometries, taking advantage of new HPC environments.

<https://github.com/NREL/BDEM/>

LIGGGHTS-INL—an adaptation of the LIGGGHTS open-source DEM particle simulation software that simulates complex particle interactions, particularly for biomass particle flow modeling. It can be used to simulate material flow in biomass feedstock processing equipment. <https://github.com/idaholab/LIGGGHTS-INL>

Mesoflow—a simulation tool that allows users to model heat and mass transport and chemical reaction in heterogeneous gas-solid systems such as biomass pyrolysis. It allows users to model the complex interactions between reaction and transport in real systems and is designed to use modern HPC computing platforms. <https://github.com/NREL/mesoflow>

SPRITE—the Smart Preprocessing & Robust Integration Emulator allows users to predict the PSD of knife-milled biomass using multiple models: Population Balance Model, Enhanced Deep Neural Operator (DNO+), and Physics-Informed DNO+ (PIDNO+). <https://github.com/idaholab/SPRITE>

Atomistic Biomass Model—an open-source model of the Populous secondary cell wall at atomistic detail guided by detailed solid-state NMR experiments. This is the first detailed, quantitative macromolecular model of the Populus secondary cell wall and provides insights into the arrangement and interactions of key biopolymers—cellulose, hemicellulose, and lignin. Researchers can use

this high-resolution model to perform simulation experiments exploring the behaviors of these biopolymers—for example, to develop new biomass conversion processes. https://pdb-dev.wwpdb.org/entry.html?PDBDEV_00000215

The FCIC Bioenergy Data Hub

FCIC researchers recognize that widely sharing the results of this work is a critical part of the FCIC mission. Publicly funded research must generate results that are “findable, accessible, interoperable, and reusable” (FAIR). As part of this commitment to FAIR data, not only have FCIC researchers made the majority of scientific publications available as open-source, free to download without charge, but FCIC researchers have also worked to standardize how experimental data are organized and labeled and developed a web portal for public access to FCIC data—the FCIC Bioenergy Data Hub, at <https://bioenergy.labworks.org/FCIC/>.

After an easy and free registration process, external stakeholders can browse through the results of FCIC research and download datasets of interest. Users can quickly identify the researchers responsible for the datasets, allowing them to reach out directly to find more information. This approach to data sharing will maximize the impact of FCIC research and lead to impactful collaborations in the future—there is often no better approach to stimulating collaborations than sharing robust data.

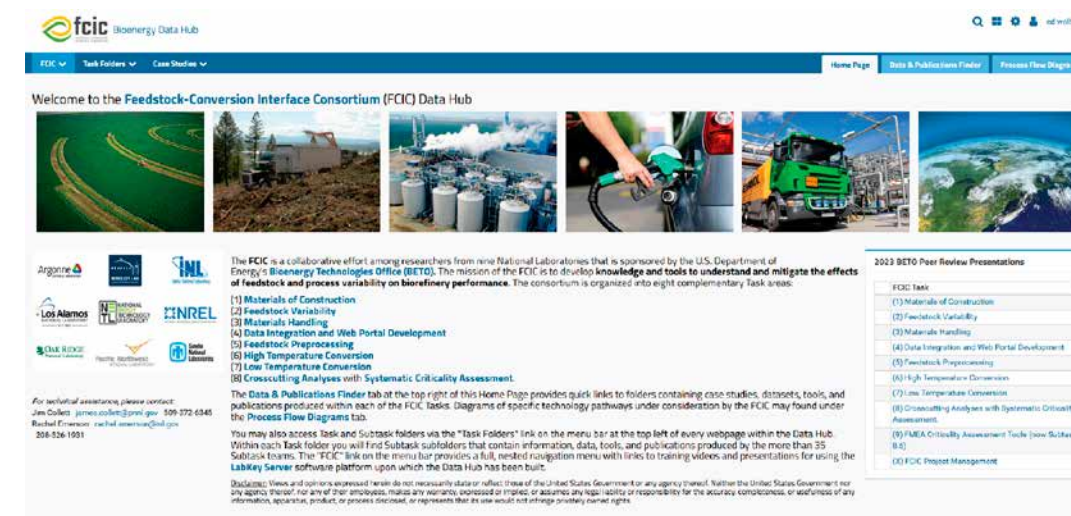


Figure 16. The FCIC Bioenergy Data Hub allows users to browse the results of FCIC research and download datasets of interest, fostering transparency and collaboration in the bioenergy community and maximizing the impact of FCIC research.

Cooperative Research and Development Agreement Projects

The FCIC has sponsored two CRADA calls to provide direct technical assistance to industry stakeholders. These calls have funded industrial projects focused on addressing the critical issue of biomass feedstock variability across the bioenergy value chain.



Idaho Forest Group (ifg.com)

Developing real-time, dynamic biomass dryer control algorithms to respond to biomass feedstocks with varying moisture contents

forestconcepts

Forest Concepts (forestconcepts.com)

Mitigating material wear issues in commercial rotary shear grinders used for biomass comminution

theWonderfulcompany™

The Wonderful Company (www.wonderful.com)

Designing robust feeding systems for small-scale gasifiers processing agricultural waste feedstocks



Jenike & Johansen (jenike.com)

Designing “smart” biomass transfer chutes with in-line acoustic sensors to monitor and mitigate variability in biomass feedstocks



Alder Renewables (www.alderrenewables.com)

Understanding the feedstock flexibility of the Alder Renewable Crude (ARC) process by detailed laboratory characterization of ARC samples produced from various feedstocks



AMP (ampsortation.com)

Characterizing how organic materials recovered from MSW streams perform during preprocessing and high-temperature thermochemical conversion



Warren & Baerg (www.warrenbaerg.com)

Developing and testing a new deconstruction head for processing landfill-bound residue bales from commercial recycling facilities



Rawlings Manufacturing (rawlingsmanufacturing.com)

Improving the durability and efficiency of commercial wood grinders by understanding and mitigating wear issues



Novastus (novastus.com)

Developing a computational model of a low-energy dryer for MSW processing to understand the impact of MSW variability on dryer performance



VERDE Nanomaterials (www.verdenano.com)

Supporting process development for a novel biomaterial made from waste biomass feedstocks with variable properties



West Biofuels (www.westbiofuels.com)

Providing detailed information on the impact of biomass feedstock variability on the performance of a novel fluidized-bed gasifier

Community Outreach

FCIC researchers have made concerted and deliberate efforts to ensure that diverse communities can participate in and benefit from their work. This has been accomplished through several deliberate outreach activities. Here are just a couple of examples:

- INL hosted a STEM event in early 2024—the Hopper Challenge—involving teams from a local rural high school.³³ The challenge was to design and build machines costing less than \$2,000 that could grind biomass. The machines were evaluated by experts from the Energy Systems Laboratory at the INL, and the winning team received a grand prize of \$3,000. The student teams—with interests in STEM—not only learned about bioenergy but also learned about working at a national laboratory.
- NREL and Metropolitan State University (MSU) in Denver, Colorado, signed a memorandum of understanding (MOU) in 2023.³⁴ MSU is an urban university with a diverse student population. Its mission is to provide a high-quality, accessible, enriching education that prepares students for successful careers, postgraduate education, and lifelong learning in a multicultural, global, and technological society. The NREL members of the FCIC were instrumental in initiating this partnership, which formalized an existing relationship among MSU faculty and students and NREL scientists and will foster even more connections going forward. The MOU is already paying dividends. In 2024, the DOE and NREL-sponsored Colorado Science Bowl³⁵ was held at MSU for the first time, exposing high school students interested in STEM to a university setting.



³³ <https://inl.gov/feature-story/rigby-students-compete-in-hopper-challenge/>

³⁴ <https://red.msudenver.edu/2023/partnership-expands-pathway-to-careers-in-renewable-energy/>

³⁵ <https://www.nrel.gov/news/features/2024/nrel-msu-denver-partnership-elevates-colorado-high-school-science-bowl-new-heights.html>

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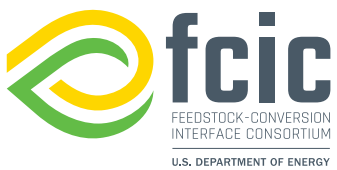
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