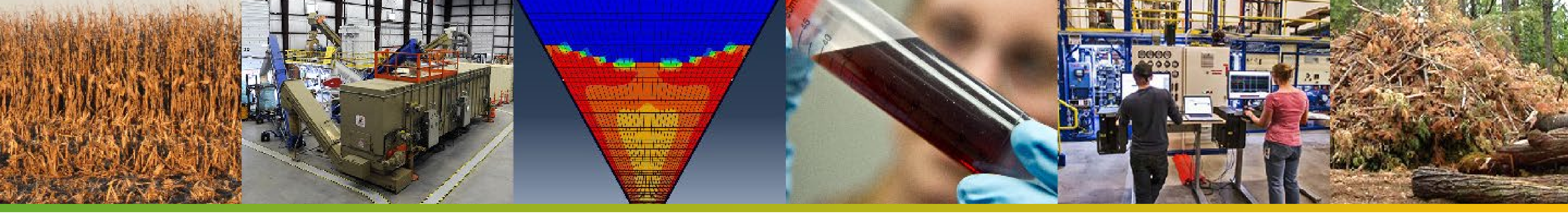

Feedstock-Conversion Interface Consortium

Edward J. Wolfrum, Ph.D.
Principal Investigator

December 9th, 2020

1-slide guide to the FCIC

The Feedstock-Conversion Interface Consortium is led by DOE as a collaborative effort among researchers from 9 National Labs

Key Ideas

- Biomass feedstock properties are **variable** and **different** from other commodities
- **Empirical** approaches to address these issues have been **unsuccessful**

We are developing **first-principles** based knowledge and tools to **understand** and **mitigate** the effects of biomass feedstock and process **variability** on biorefineries

Sandia National Laboratories
Argonne National Laboratory
INL Idaho National Laboratory
Pacific Northwest National Laboratory
Oak Ridge National Laboratory
Berkeley Lab
National Energy Technology Laboratory
NREL National Renewable Energy Laboratory
Los Alamos National Laboratory

1-slide guide to the FCIC

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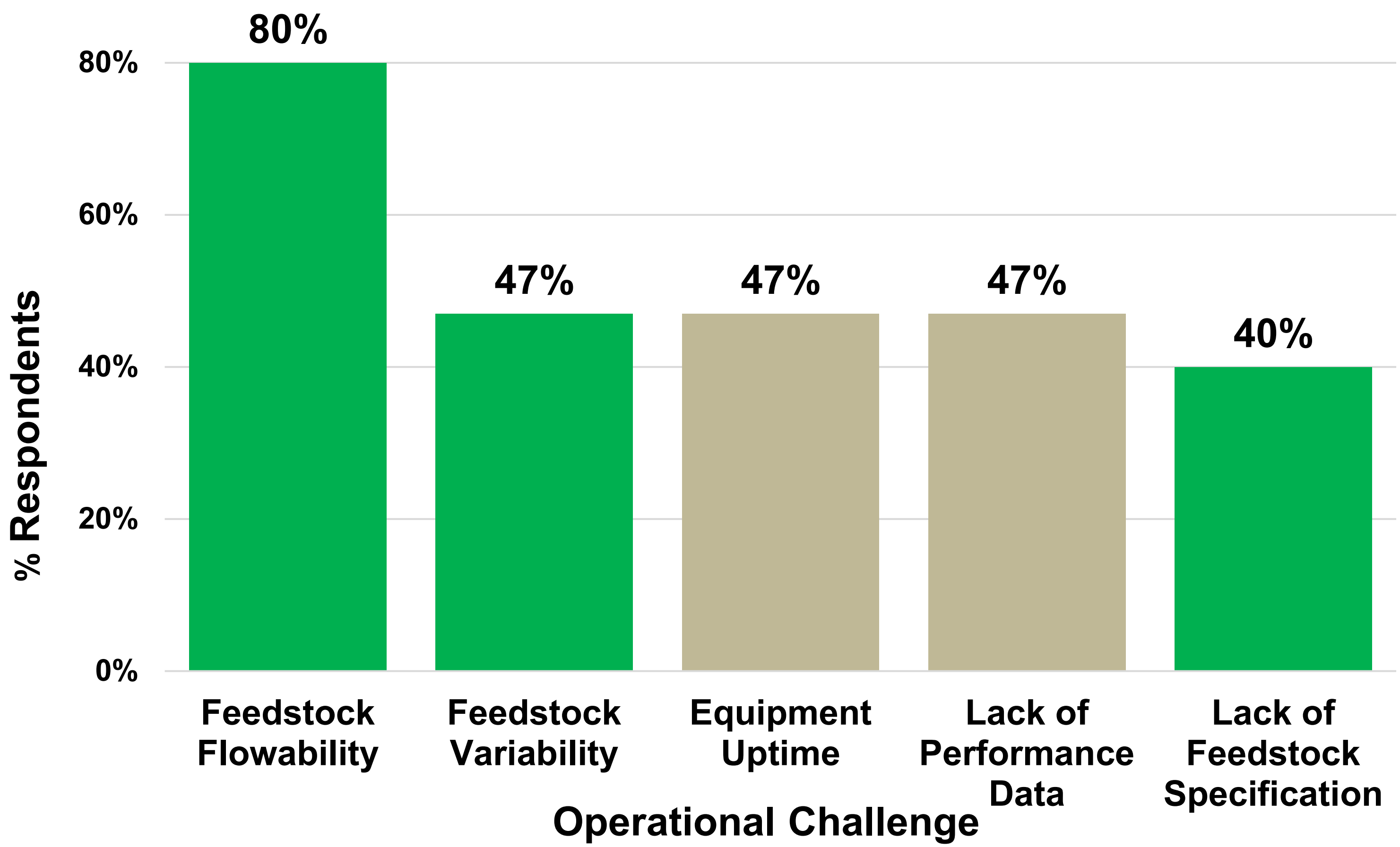
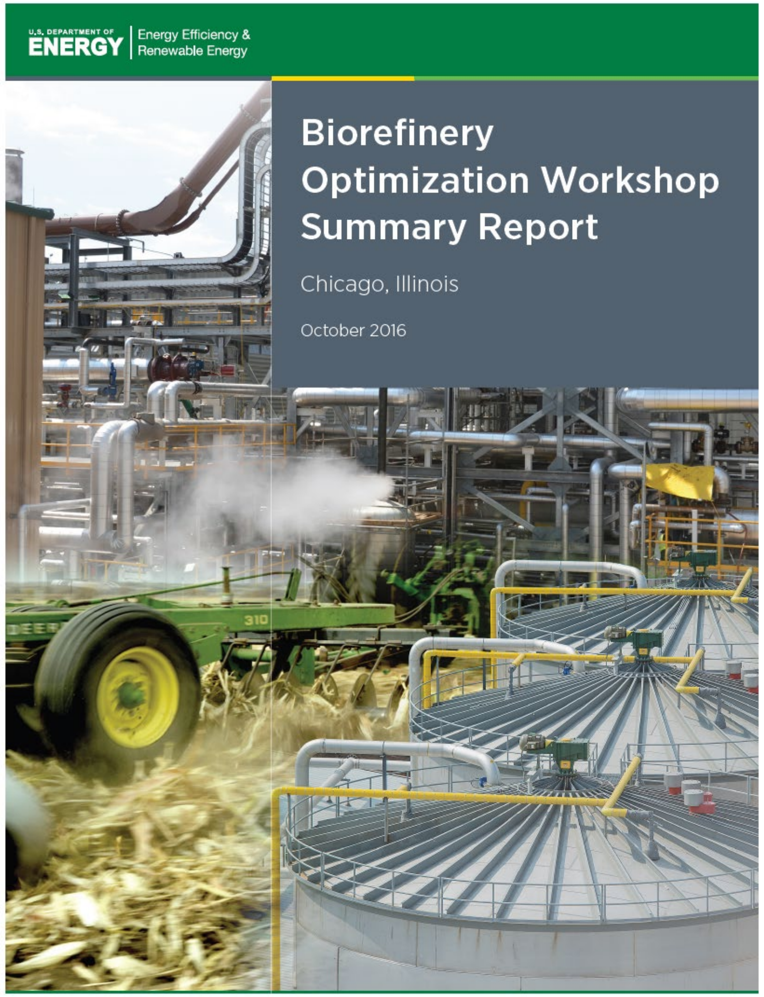
2016 Biorefinery Optimization Workshop

- Challenges, recommendations, and lessons learned from over 100 participants (industry, NL, academic)

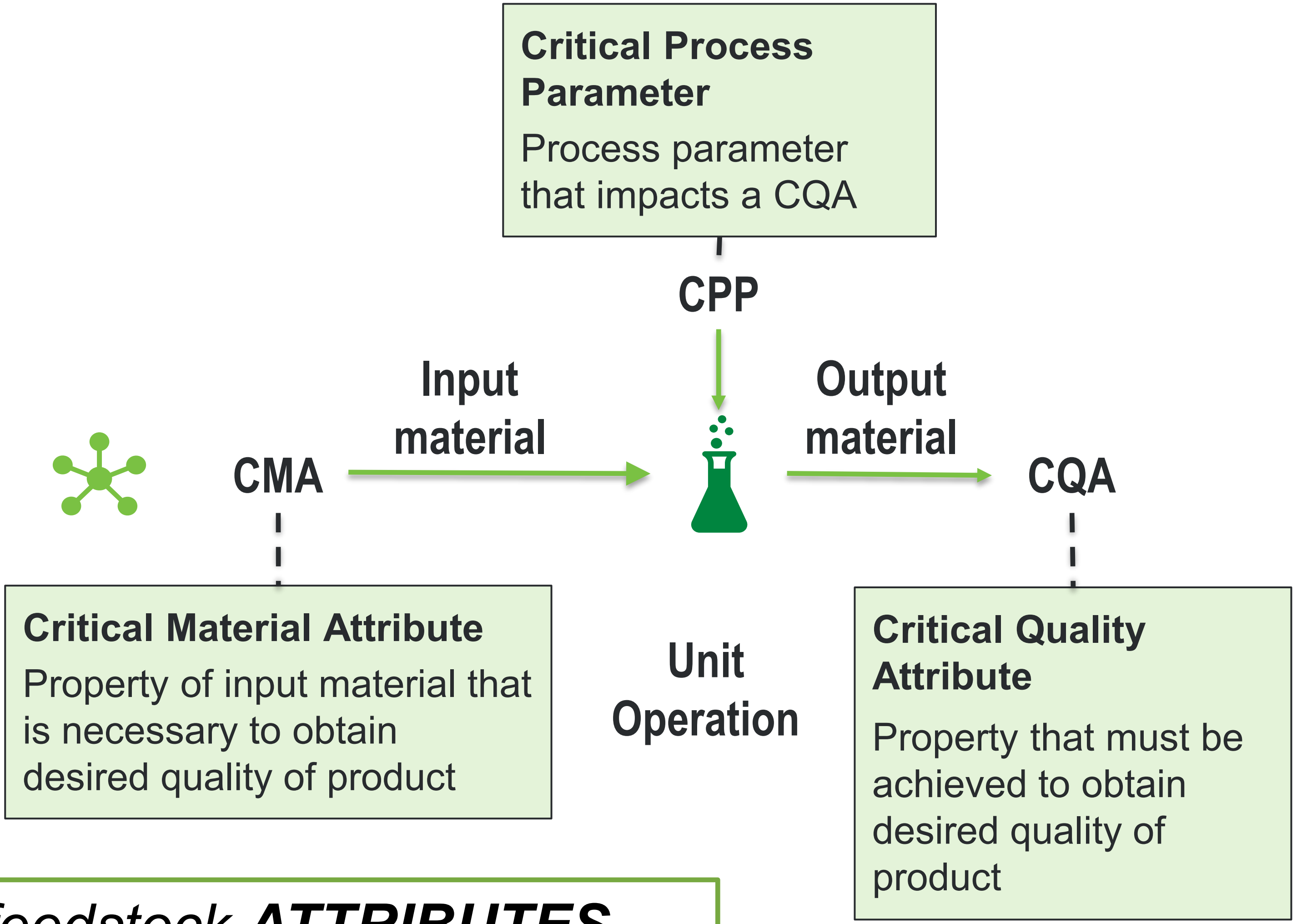




https://energy.gov/eere/bioenergy/downloads/biorefinery-optimization-workshop-summary-report

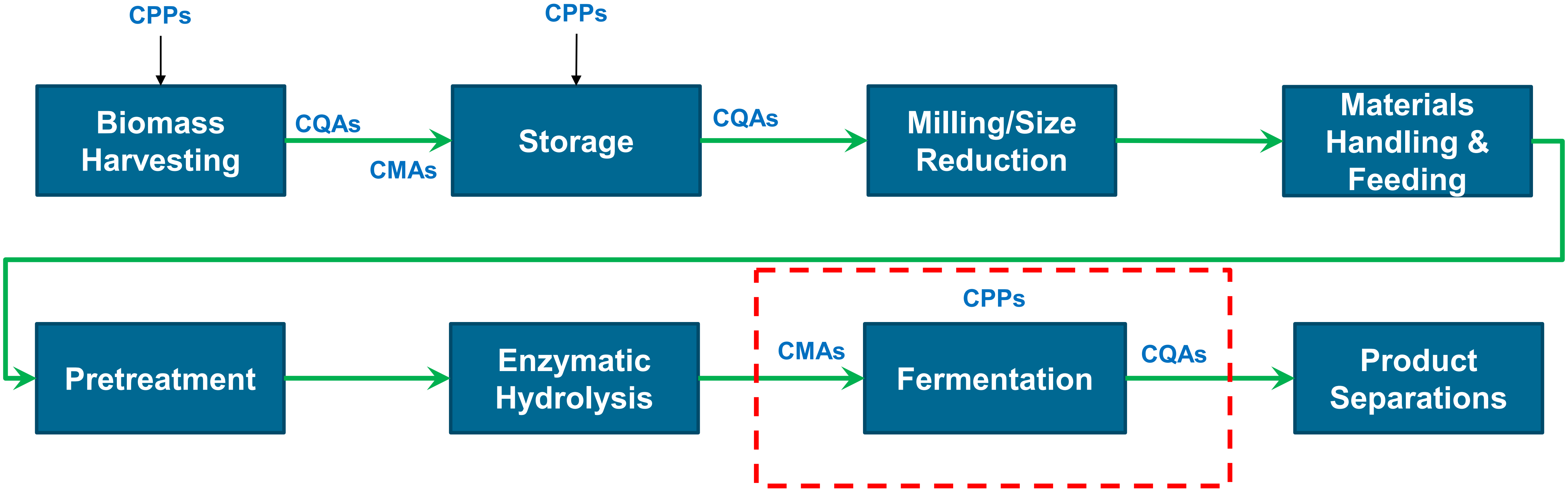
Quality by Design (QbD)

- Key operating concept and organizing principle
- Widely used in pharmaceutical manufacturing – FDA-endorsed
- Chemical processes are collections of specific unit operations
- Unit operations are discrete but connected



*Moving from feedstock **NAMES** to feedstock **ATTRIBUTES***

QbD for the Biomass Value Chain



CMAs:
Monomeric sugar content
Pretreatment byproducts
Inorganics (e.g. Na, K)

CPPs:
Temperature
Feeding strategy
Media composition

CQAs:
Product TRY
- Rate, titer, yield

Residual substrate
Byproducts

Eight Tasks Working Across the Value Chain

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Feedstock → **Preprocessing** → **Conversion**

Feedstock Variability:
Develop tools that quantify & **understand the sources of biomass resource and feedstock variability**

Preprocessing:
Develop tools to enable technologies that **provide well-defined and homogeneous feedstock** from variable biomass resources

Conversion (High & Low-Temperature Pathways):
Develop tools to enable technologies that **produce homogeneous intermediates** that can be converted into market-ready products

Materials Handling:
Develop tools that enable continuous, steady, trouble free feed into reactors

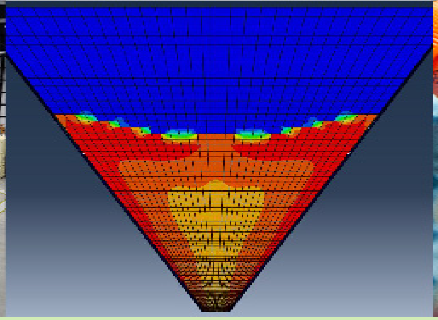
Materials of Construction:
Develop tools that **specify materials** that do not corrode, wear, or break at unacceptable rates.

Enabling Tasks

Scientific Data Management: Ensure the data generated in the FCIC are **curated and stored** – FAIR guidelines

Crosscutting Analyses TEA/LCA:
Works with other Tasks **enable valuation** and intermediate streams and quantify impact of variability.






Task Highlights

FCIC
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Feedstock Variability Task

Objective:

- Identify & quantify the initial distribution of feedstock CMAs and inform strategies to reduce and manage this variability

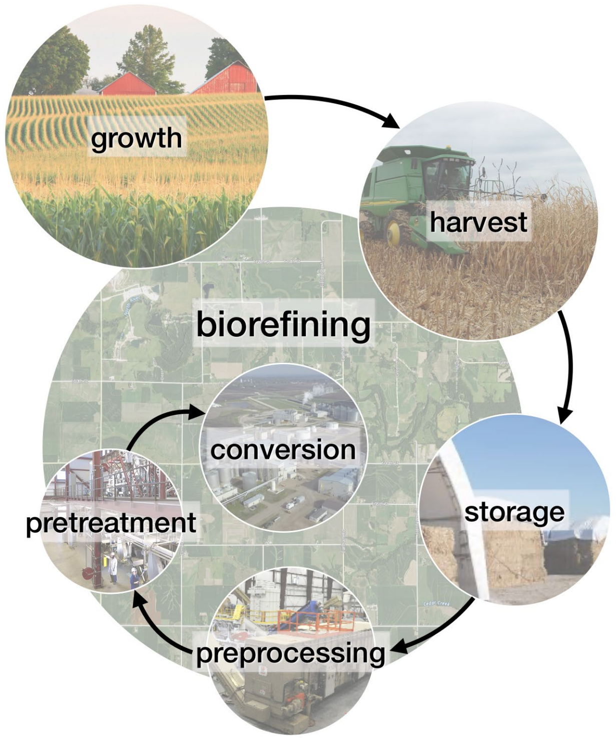
Impact:

- Characterization tools and CMA variability data that inform 1) storage and harvest best practices, 2) feedstock quality, and 3) selection of process configurations that manage variability from field through conversion
- Feedstock suppliers, process designers, equipment manufacturers, & investors will derive value from this fundamental knowledge of economic drivers that are critical to de-risking the industry

Outcome:

- Understanding of key sources of biomass variability (e.g., storage degradation, harvest conditions, anatomical fractions, genetics, location) to identify and quantify CMA distributions that propagate across unit operations to inform cost-effective management of variability across the value chain.

feedstock variability

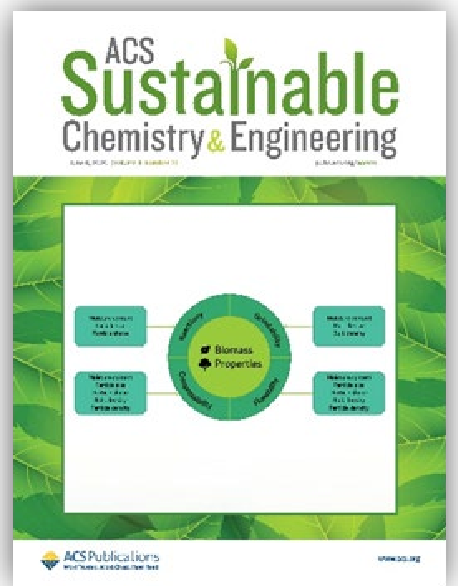


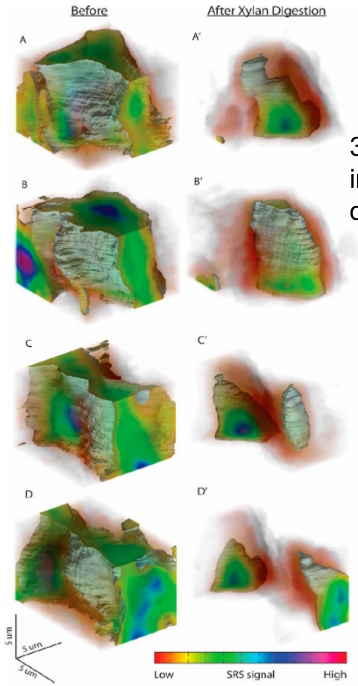
Characterizing variability in lignocellulosic biomass

Knowledge

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Provided a critical review of advanced methods for characterizing feedstock variability





3D chemical imaging of xylan digestion

Current Knowledge Gap

- Feedstock variability is a significant barrier to the scale-up and commercialization of lignocellulosic biofuel technologies
- Variability in feedstock characteristics and behavior creates challenges to the biorefining industry by affecting continuous operation and yields

Achievement

- We reviewed several advanced analytical methods that measure density, moisture content, thermal properties, flowability, grindability, rheology properties, and micromorphology
- We examined methods that have not traditionally been used to characterize lignocellulosic feedstocks but have the potential to bridge the gap in our explanation of feedstock variability

Relevance

- Currently, feedstock variability is understood and explained largely based on chemical composition
- Physical and mechanical properties and behavior of lignocellulosic feedstock in various unit operations, studied through advanced analytical methods, can further explain variability

"Characterizing Variability in Lignocellulosic Biomass: A Review", Jipeng Yan, Oluwafemi Oyedeji, Juan H. Leal, Bryon S. Donohoe, Troy A. Semelsberger, Chenlin Li, Amber N. Hoover, Erin Webb, Elizabeth A. Bose, Yining Zeng, C. Luke Williams, Kastli D. Schaller, Ning Sun, Allison E. Ray, and Deepti Tanjore
ACS Sustainable Chemistry & Engineering 2020 8 (22), 8059-8085, DOI: 10.1021/acssuschemeng.9b06263

Characterizing bale degradation

Knowledge

Identified and quantified hemicellulose modification due to biological degradation using analytical pyrolysis and multidimensional GCMS

Current Knowledge Gap

- Biomass degradation during long-term storage negatively affects conversion performance (and value) of the biomass
- There has been limited success in quantifying degradation beyond qualitative visual inspection

Achievement

- We used py-GC/GC to identify and quantify breakdown products in corn stover samples with different biological degradation profiles
- The findings suggest that biological heating disrupts cell wall structure, fragmenting the hemicellulose or cellulose chains

Relevance

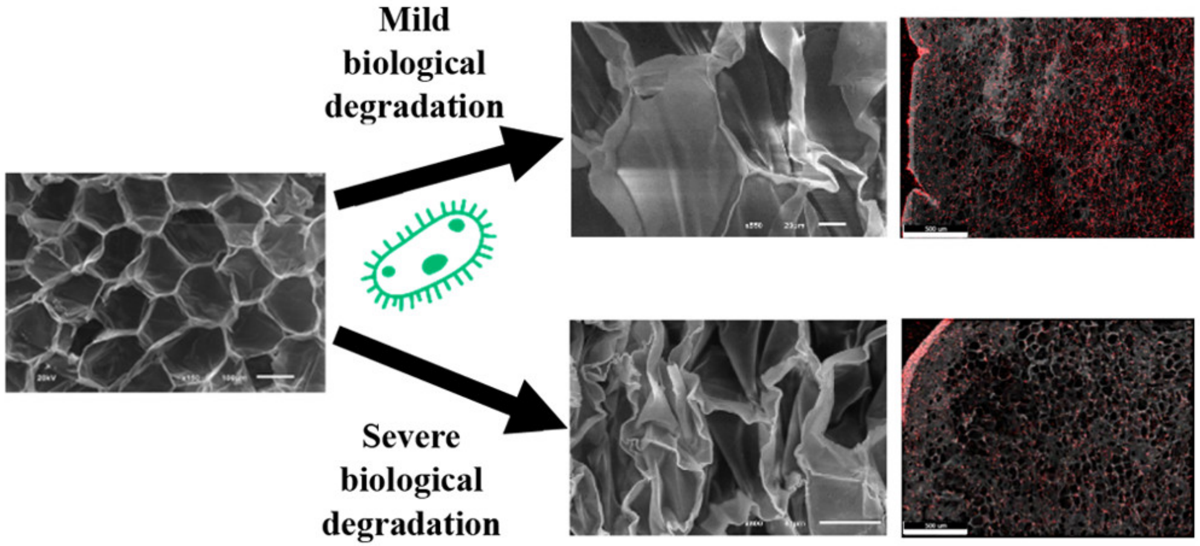
- Stakeholders can use this technique to rapidly characterize biomass feedstock degradation and correlate with downstream conversion performance
- FCIC researchers were invited by the py-GC/GC instrument manufacturer (LECO) to present the work in an upcoming conference (Spring 2021)

Signatures of Biologically Driven Hemicellulose Modification Quantified by Analytical Pyrolysis Coupled with Multidimensional Gas Chromatography Mass Spectrometry
Gary S. Groenewold, Brittany Hodges, Amber N. Hoover, Chenlin Li, Christopher A. Zarzana, Kyle Rigg, and Allison E. Ray
ACS Sustainable Chemistry & Engineering 2020 8 (4), 1989-1997, DOI: 10.1021/acssuschemeng.9b06524

Characterizing inorganic species variability in corn stover fractions

Knowledge

Characterized cell wall structure and localized inorganic species variability in harvested and stored corn stover fractions



Current Knowledge Gap
- Conventional approaches of evaluating inorganics impacts are based on a total ash content of bulk materials with little tracking or understanding of the fate, form, and impacts of individual species.
- Natural variability in inorganic species at anatomical and tissue scales have been overlooked.

Achievement
- Conducted a first-of-a-kind study on the dynamic elemental variability and distributions observed in corn stover fractions as functions of storage and biological heating.
- Inorganic species mapping of corn stover stems suggested that biological heating and degradation resulted in translocation of silica from the pith to the outer epidermal tissues.

Relevance
- Provides fundamental understanding to inform strategies for harvest and collection, abrasive wear mitigation, selective biomass preprocessing technologies, and equipment design.

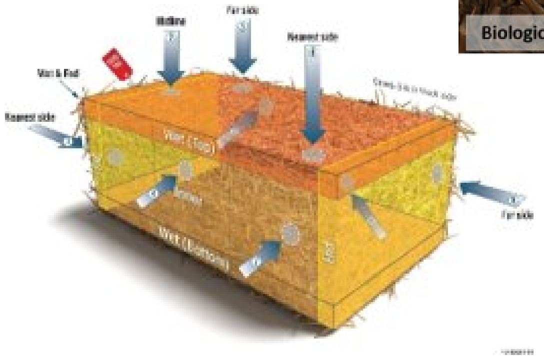
"Characterization and Localization of Dynamic Cell Wall Structure and Inorganic Species Variability in Harvested and Stored Corn Stover Fractions as Functions of Biological Degradation", Chenlin Li, Patricia Kerner, C. Luke Williams, Amber Hoover, and Allison E. Ray, ACS Sustainable Chemistry & Engineering 2020 8 (18), 6924-6934, DOI: 10.1021/acssuschemeng.9b06977

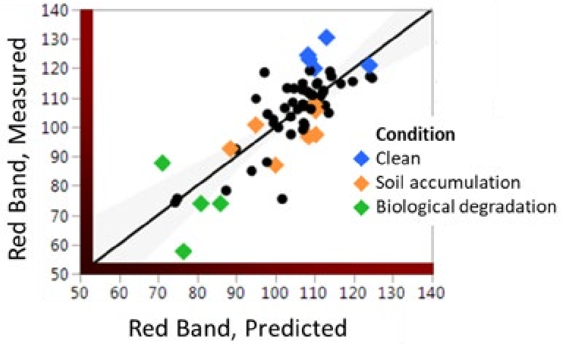
Image analysis of biomass: quality assessment in RGB color space

Tools

Image analysis for rapid assessment and sorting of corn stover/pine based on material attributes

Corn Stover Bale





Description

- Analysis of bale core images differentiates sample quality into soil-contaminated, biological degradation, or clean fractions
- 72% of the measured variability in red band in the images was explained by SiO2 and glucan content
- Work to analyze broader FCIC soil contaminated and biologically degraded corn stover sample sets is in progress
- Images are available to augment datasets to support subtask 5.5 machine vision work for quality identification

Value of new tool

- Enables process control/optimization by providing foundational information for sorting corn stover/pine based on material attributes

Potential Customers & Outreach Plan

- Promise for development of a rapid screening tool that could be deployed by farmers for in-field assessment or by operators for in-line process measurement and downstream controls/optimization

Multiscale Characterization of Lignocellulosic Biomass Variability and Its Implications to Preprocessing and Conversion: a Case Study for Corn Stover
Allison E. Ray, C. Luke Williams, Amber N. Hoover, Chenlin Li, Kenneth L. Sale, Rachel M. Emerson, Jordan Klinger, Ethan Oksen, Akash Narani, Jipeng Yan, Christine M. Beavers, Deepti Tanjore, Manal Yunes, Elizabeth Bose, Juan H. Leal, Julie L. Bowen, Edward J. Wolfrum, Michael G. Resch, Troy A. Semelsberger, and Bryon S. Donohoe
ACS Sustainable Chemistry & Engineering 2020 8 (8), 3218-3230, DOI: 10.1021/acssuschemeng.9b06763

Material Handling Task

Objective: Develop first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat.

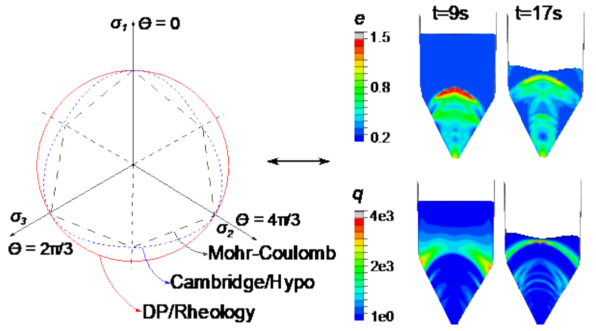
Impact:
- This task provides industry with characterization tools and CMA variability data that inform 1) storage and harvest best practices, 2) feedstock quality, and 3) selection of process configurations that manage variability from field through conversion
- Feedstock suppliers, process designers, equipment manufacturers, & investors will derive value from this fundamental knowledge of economic drivers that are critical to de-risking the industry

Outcome:
- First principles-based design tools derived from validated models for equipment designers to ensure reliable continuous bulk solids handling and transport. Identify the safe and reliable working envelope of CMAs, CQA for achieving CPP's (i.e. design charts for consistent flow)
- Open-source constitutive models as ABQUS FEM and OpenFOAM FVM modules

Potential Customers & Outreach Plan:
- Publications of peer-reviewed scientific journals (with open access whenever possible) to promote knowledge, tools and collaborations
- Open-source strategy in flow simulators, experimental data and design charts to attract investors, process designers, equipment manufactures
- CRADA projects between industry and labs to enable simulations on HPC

of arbitrary shapes

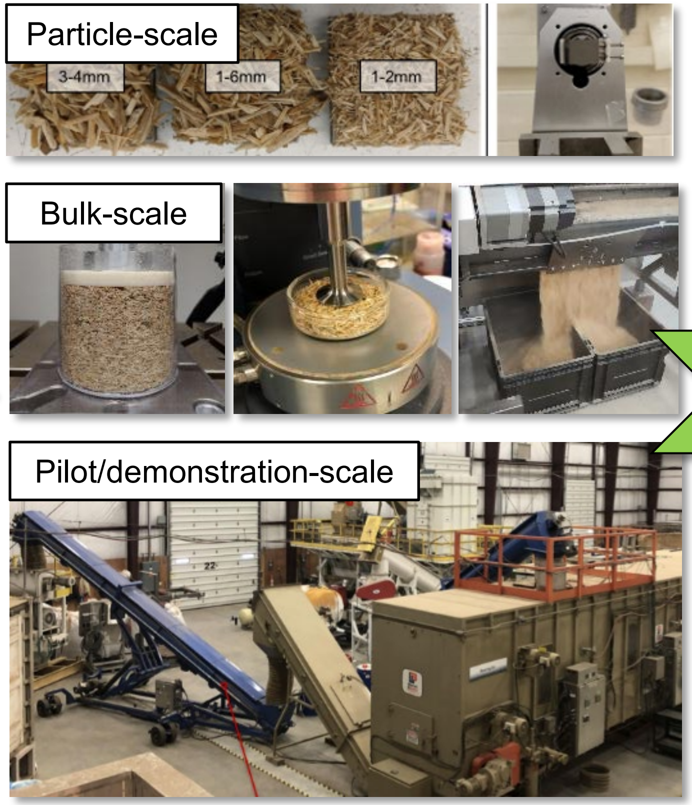
A v-shape hopper discharge simulation



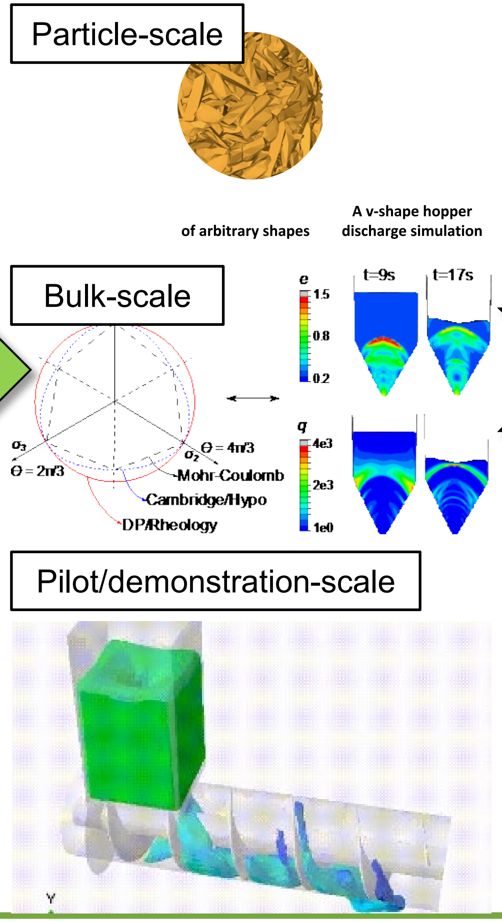
Materials Handling Task

Process upsets in handling are a major challenge for lowering costs of biomass. Solutions?

Experimental: multi-scale material characterization for state-of-the-art **knowledge** and **design charts**



Computational: experiment-validated multi-scale biomass mechanics & flow simulators as **open-source toolkits**



Outcome: efficient & effective design charts and simulators for bioenergy industries and other applicable areas

Preprocessing
CQAs (e.g. particle shape, PSD, feed rate)

CMAs & CPPs (e.g. particle shape, PSD, feed rate)
Material Handling
CQAs (controlled flow rate)

CMAs & CPPs (e.g. particle shape, PSD, feed rate)
Conversion
CQAs

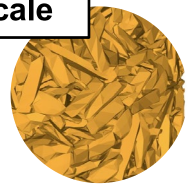
Flow models: Limitations & best practices

Knowledge

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Identified particle- & bulk-scale models suitable for the flow of milled biomass and recommended best practices

Particle-scale

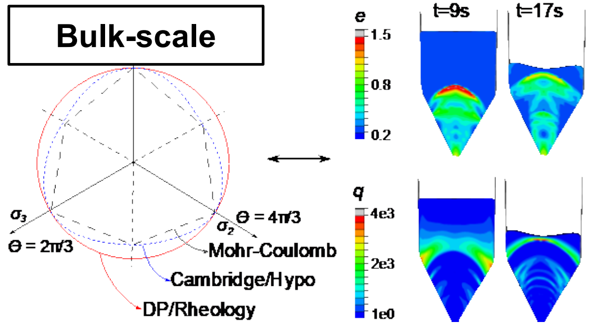


of arbitrary shapes

A v-shape hopper discharge simulation

A review of computational models for the flow of milled biomass I: Discrete-particle models, *ACS Sustainable Chemistry & Engineering*, 8, No. 16 (2020): 6142-6156. https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.0c00402

Bulk-scale



A review of computational models for the flow of milled biomass II: Continuum-mechanics models, *ACS Sustainable Chemistry & Engineering*, 8, No. 16 (2020): 6157-6172. https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.0c00412

Current Knowledge Gap

- Lack of computational models suitable for the flow of milled biomass
- Lack of experimental data for supporting the development of new models
- Lack of open-source model development platforms for user coverage

Achievement

- Assessed and identified limitations of existing models as knowledge base
- Recommended potential flow models and codes for biomass materials
- Demonstrated early progress for proof of evidence and best practices

Relevance

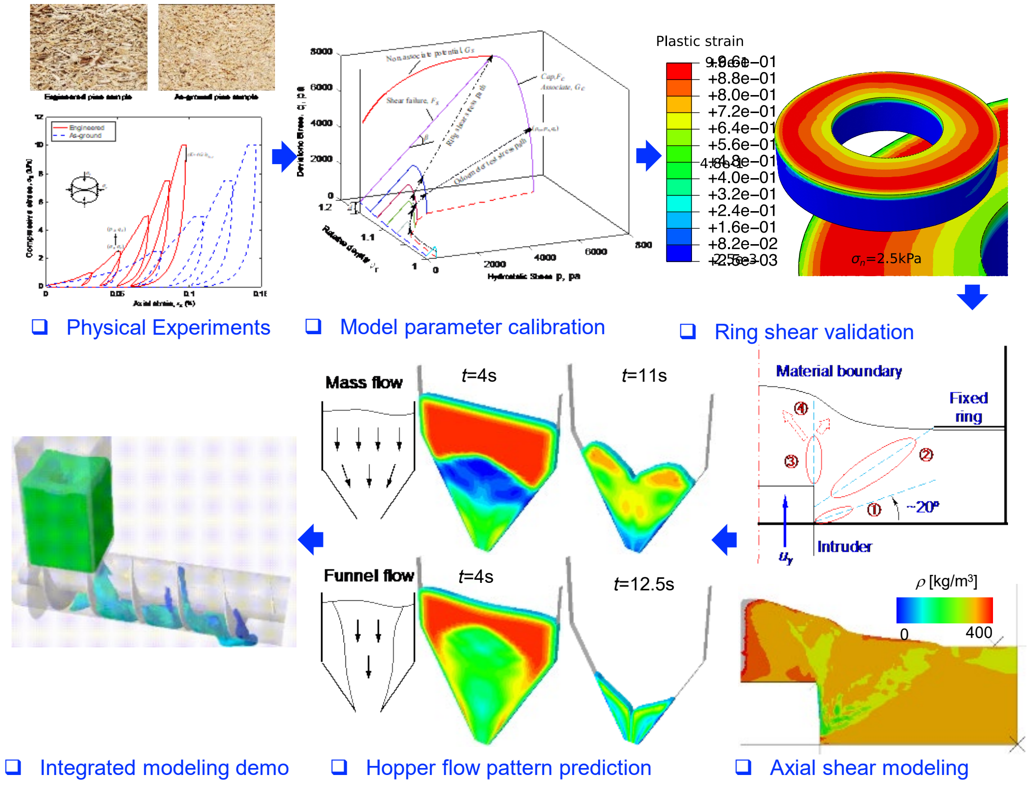
- Stakeholders within the bioenergy industry and academic communities will avoid wasting investment in modeling techniques not suitable for biomass
- FCIC researchers were invited to give multiple presentations at ASABE AIM (Summer 2020) to present the experience of biomass model development
- FCIC researchers were invited to lead panel discussion at the International Powder & Bulk Solids Conference and Exhibition (Fall 2020) and interface with industry experts in this area [conference postponed to early 2021]

Continuum-mechanics based flow models

Tools

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Implemented and reformulated advanced continuum particle flow models to predict feedstock flow across scales and regimes



- *A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine, Powder Technology*, 368:45-58, 2020. https://doi.org/10.1016/j.powtec.2020.04.038
- Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model, Energy, under review, 2020.

Description

- Implemented and applied four advanced continuum particle flow models with physical experiment-based calibration for biomass granular material
- Validated, down-selected, and reformulated one constitutive model to accurately capture the flow behavior at both the quasi-static and the dense flow regimes through multi-scale shear/hopper testers

Value of new tool

- The flowability issues (equipment jamming/plugging, etc.) in biorefineries are due to poor understanding of feedstock flow physics.
- Simulation at industry scale using the constitutive model will identify the CMAs that control material flow and provide a tool to optimize equipment design and to guide equipment operation for biorefinery engineers
- Sensitivity analysis using the constitutive model will provide CMAs working envelops for conventional flow equipment as a tool and the tool will guide biomass preprocessing steps

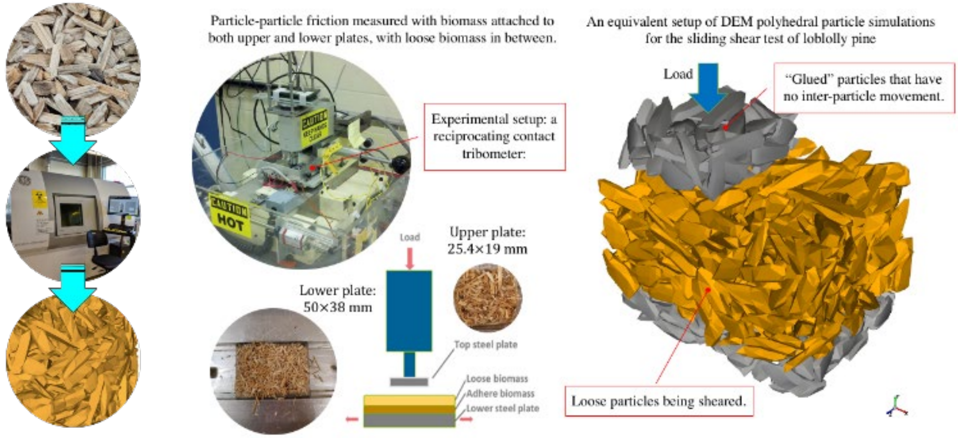
Potential Customers & Outreach Plan

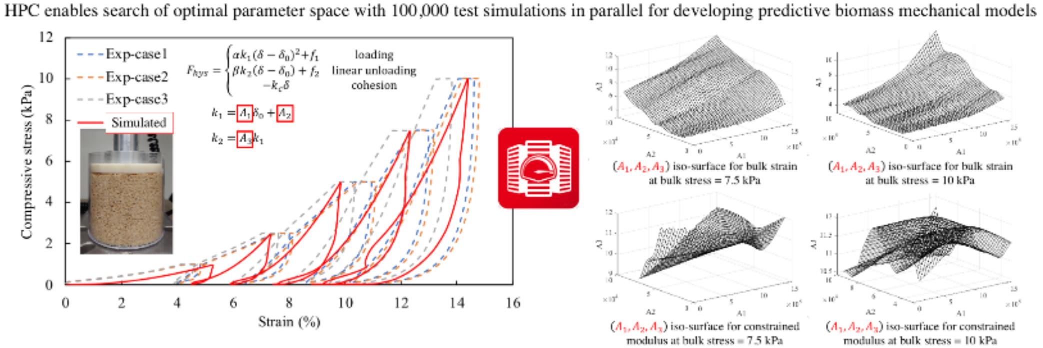
- Biomass feedstock handling equipment suppliers, biorefinery designers
- Open-source continuum mechanics models offered for public use

DEM for fundamental particle physics

Tools

Developed XCT-informed polyhedral DEM for fractured pine particles and HPC-enabled open-source coarse-grain DEM for accurate contact physics





Description

- Developed XCT-informed DEM simulation workflow for quantifying the influence of particle shape and size as CMAs in compression & shear
- Developed coarse-grain DEM with semi-empirical mechanistic contact laws and implemented in an HPC-enabled open-source package

Value of new tool

- The first-of-its-kind virtual laboratory for biomass particle mechanics
- The open-source strategy maximizes flexibility of DEM development
- A fundamental and low-learning-curve design tool for industries
- Potential to be further developed as a cloud-based characterization tool

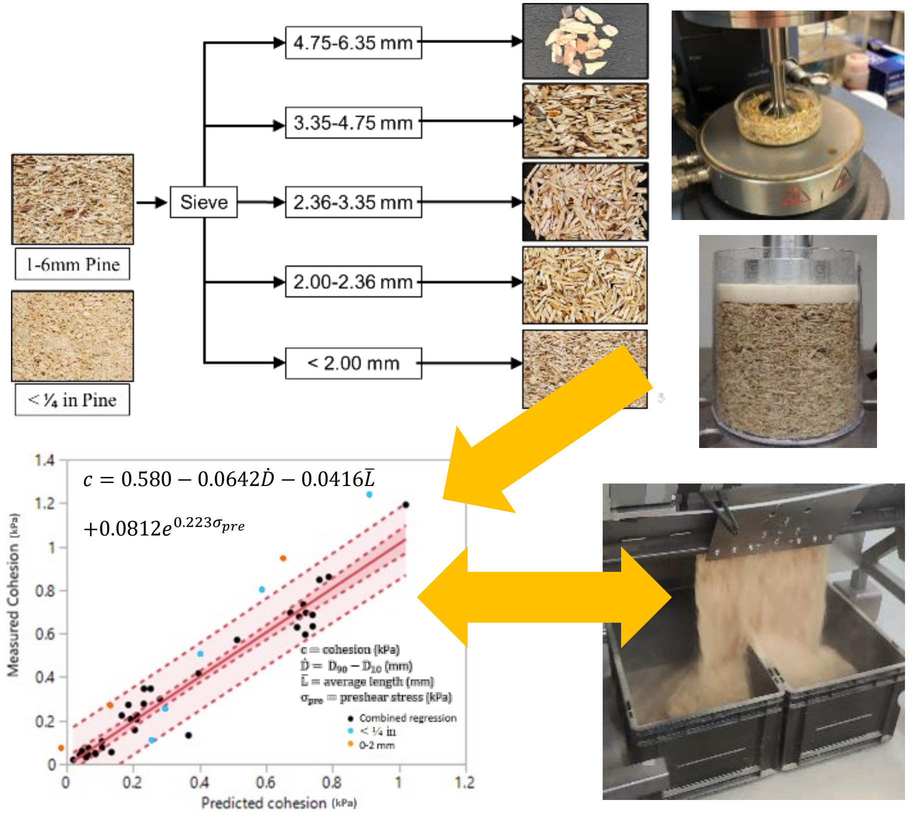
Potential Customers & Outreach Plan

- Biomass feedstock handling equipment suppliers, biorefinery designers
- Bulk solids handling consulting and design companies
- Academic communities for fundamental scientific studies

Multiscale bulk flow characterization

Knowledge

Developed relationships between material attributes and resulting shear and bulk flow properties.



Current Knowledge Gap

- Current state-of-the-art particle mechanics and granular flow models were developed in soil mechanics with test methods appropriate for incompressible, regular solids.
- These test methods do not directly extract equivalent properties for biomass because of the complex interactions of biomass anisotropic compressibility, bulk creep, surface properties and morphology, and heterogeneity/variability.
- Current quasi-static test methods and properties do no directly predict or indicate flow performance in pilot equipment such as has been developed for powders and soils.

Achievement

- Develop multiscale characterization methods and pair with flow validation data to correlate material attributes with bulk flow performance, and lab-scale flow inception and critical state shear properties.

Relevance

- Understanding how characterization methods and material properties impact flow performance will allow for better materials characterization by academia and industrial stakeholders, as well as more robust testing and equipment design for broad bioenergy feedstock.

Preprocessing Task

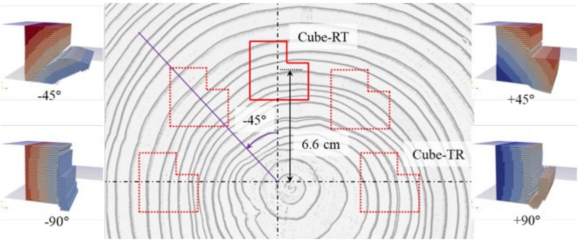
Objective: Develop science-based design and operation principles informed by TEA/LCA that result in predictable, reliable and scalable performance of preprocessing unit operations.

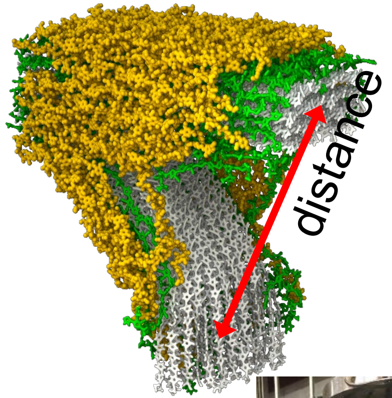
Impact: This task will provide knowledge and tools to pioneer biorefineries and other industry stakeholders through fundamental studies of comminution, fractionation, and deacetylation that produce validated mechanistic models.

Outcome: A first-principles-based set of modeling tools that predict how material attributes of corn stover and pine residues and process parameters of milling, size classification and deacetylation unit operations interact to produce feedstocks with quality attributes required by downstream conversion.

Potential Customers & Outreach Plan:

- Publications of peer-reviewed scientific and trade journals to promote knowledge, tools and collaborations and presentation of work at relevant conferences and trade shows
- Open-source strategy for all model codes
- Incorporate design aspects and control capabilities to mitigate feedstock variability impacts to next-generation equipment designs and share results with equipment manufacturers.

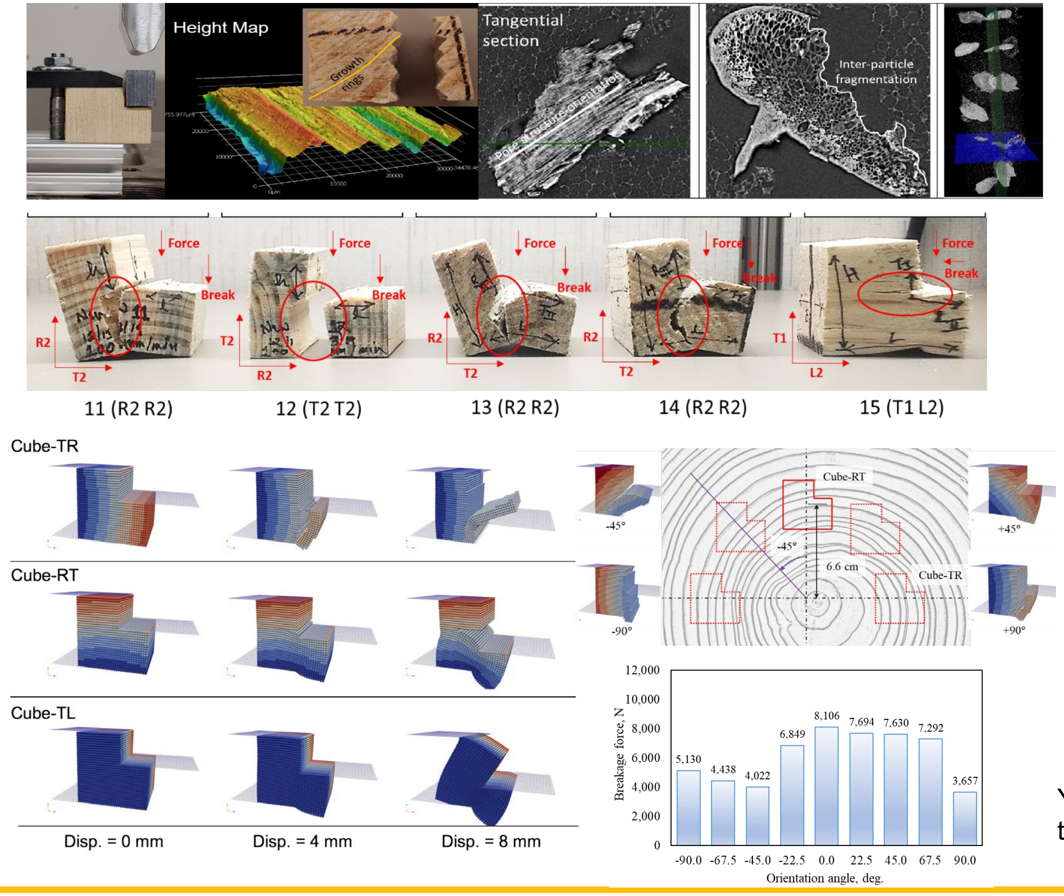




Deconstruction Mechanism Theory & Models

Tools

Developed experiment-validated open-source macroscale DEM model for pine structural deformation & deconstruction



Description

- Developed a benchmark deconstruction testing procedure for quantifying material failure and applied for pine wood block
- Characterized shear failure surface for enhanced scientific knowledge
- Developed experiment-validated open-source macroscale DEM model for pine structural deformation & deconstruction

Value of new tool

- The first-of-its-kind virtual laboratory for biomass micromechanics
- The macroscale mechanics DEM model will be open-source
- Applicable for engineering-scale equipment design and validation

Potential Customers & Outreach Plan

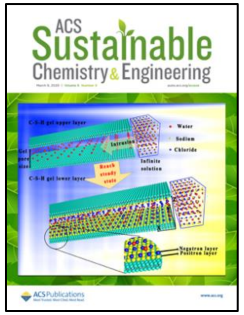
- Biomass feedstock preprocessing industry partner, biorefinery designers
- Conference presentations in FY21 (ASABE, EMI and AIChE)

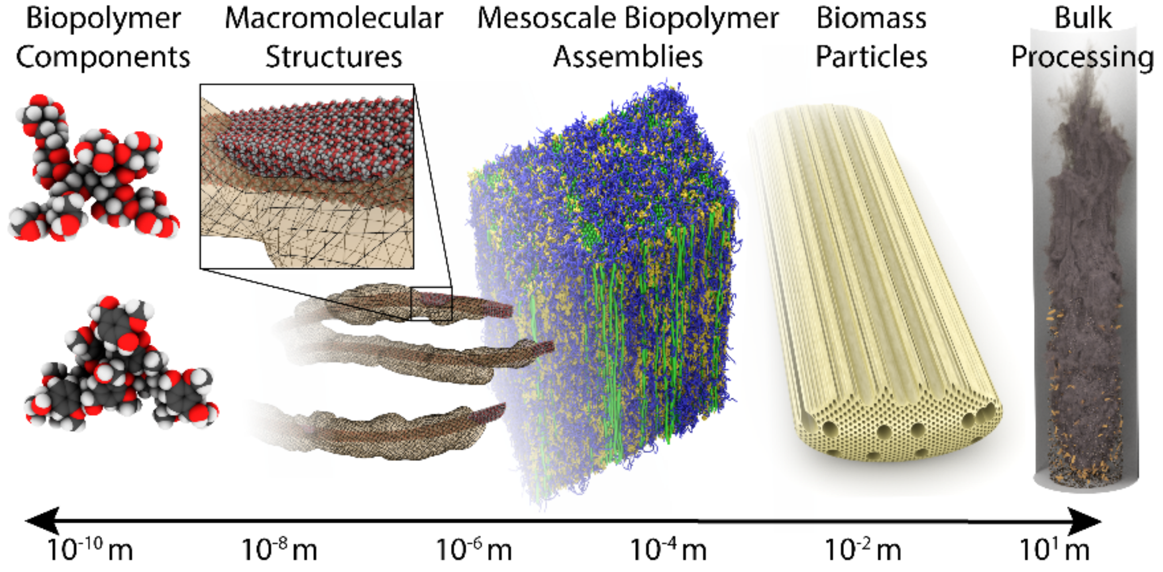
Yuan Guo, Qiushi Chen, Yidong Xia, Jordan Klinger, Vicki Thompson, “A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles,” submitted to Powder Technology (under review).

Advances in Multiscale Modeling of Lignocellulosic Biomass

Knowledge

Modeling and experimental verification across a range of biomass length scales provides a useful tool to optimize design and de-risk biorefinery operations





Peter N. Ciesielski, M. Brennan Pecha, Aaron M. Lattanzi, Vivek S. Bharadwaj, Meagan F. Crowley, Lintao Bu, Josh V. Vermaas, K. Xerxes Steirer, Michael F. Crowley. "Advances in Multiscale Modeling of Lignocellulosic Biomass." *ACS Sustainable Chemistry & Engineering* (2020) 3512-3531. https://doi.org/10.1021/acssuschemeng.9b07415.

Current Knowledge Gap

- The relationships that govern emergent properties are poorly understood and span many length scales.
- Characterization and modeling performed at a single length scale is insufficient to understand and predict behavior.

Achievement

- Coupled experimentation and modeling over a range of length scales to identify structural and compositional features that dictate emergent properties
- Provides the ability to track the impact of variability at all length scales.

Relevance

- Provides an experimentally validated tool that predicts performance of biomass feedstocks in various processing scenarios.
- Will help design and optimize biorefinery operations, de-risk deployment, and help determine the value of a feedstock as a function of CMAs.

Air Fractionation for Anatomical Separation

Tools

Anatomical separation of corn stover and loblolly pine residues using air fractionation

Description

Air fractionation system to separate materials based on buoyancy which encompasses material properties such as density, shape, surface area, size and roughness. Since different plant anatomical fractions have different values for these properties, fractions can be effectively selected and enriched

Value of new tool

Currently the entire plant is utilized and differences in material properties result in variability during grinding, conveying, pretreatment, conversion and upgrading. This tool allows anatomical fractions to be enriched so that they can be processed differently if necessary. For example, corn stalks are more recalcitrant than cobs, leaves or husks and leaves and husks tend for form bird's nest and fines during processing.

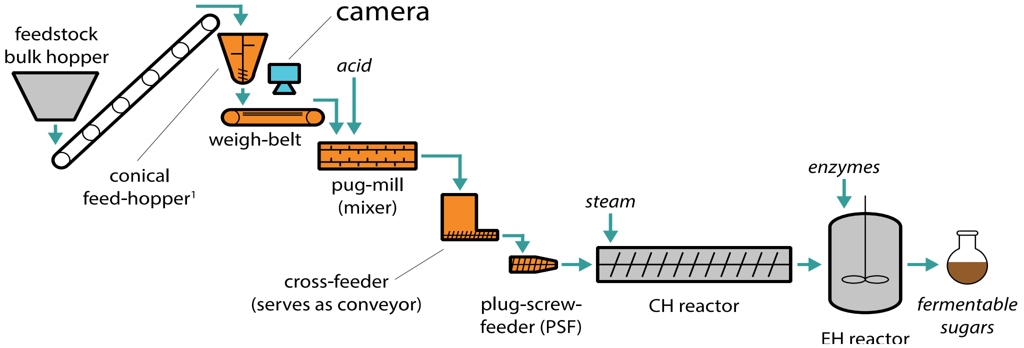
Potential Customers & Outreach Plan

Next generation biorefineries

Publish the results of experimental studies and TEA/LCA studies to demonstrate the benefits of this approach.

Real-Time Feedstock Image Analysis

Developed automated machine vision technique to measure biomass feedstock particle quality in real-time to enable advanced process control strategies



Description

- Utilized a 26,000-image dataset from a continuous weigh belt feeder to a corn stover pretreatment reactor using inexpensive digital cameras.
- Neural Network (NN) and Pixel Matrix Feature Parameterization (PMFP) approaches developed.

Value of new tool

- Neural Network (NN) models were able to predict anomalies (feed interruption, coarse-particle segregation) even when camera lens obscured by dust (97% true positive/3% false negative).
- PMFP method indicated significant textural features related to surface roughness, shade variations, and particle angular direction variations (particle size distribution variation).
- NN and PMFP approaches are complementary to one another and can describe why feedstock images are classified a certain way.

Potential Customers & Outreach Plan

- Broad applicability to other unit operations where continuous feeding images can be gathered

"Real-time biomass feedstock particle quality detection using image analysis and machine vision", Chandrakanth Gudavalli, Elizabeth Bose, Bryon S. Donohoe & David A. Sievers, Biomass Conversion and Biorefinery (2020) DOI:10.1007/s13399-020-00904-w

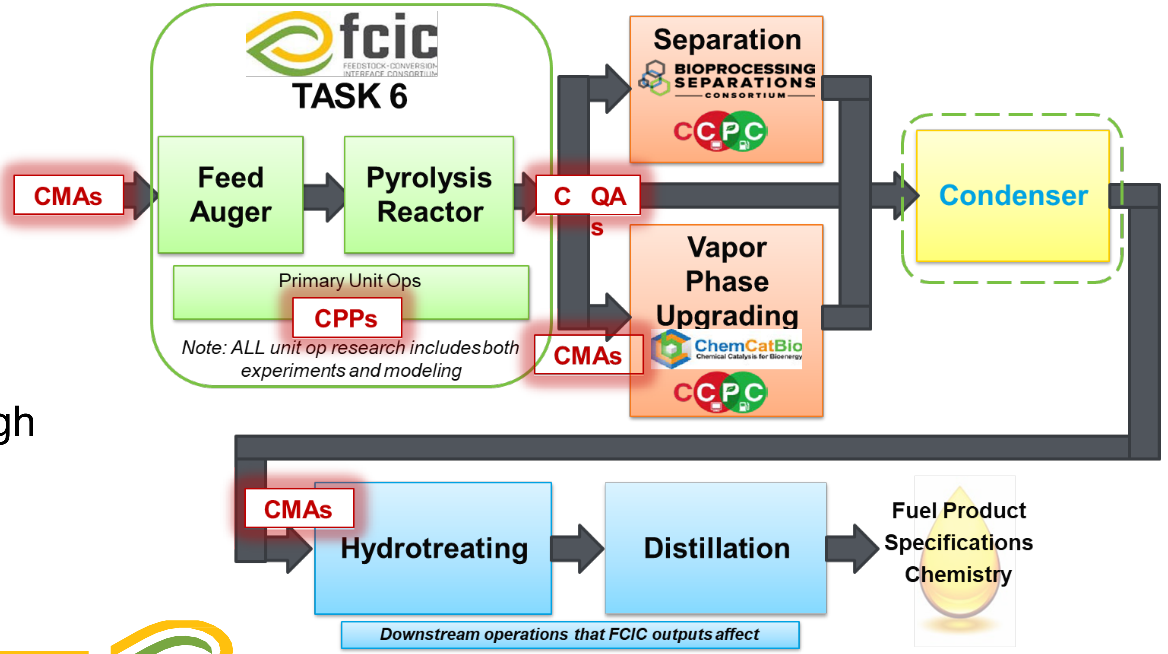
High Temperature Conversion Task

Objective: Develop the science-based understanding required to accurately predict the effects of variable feedstock attributes (CMAs) and process parameters (CPPs) on pyrolysis product quality attributes (CQAs).

Impact: Feedstock impacts on high-temperature unit operations are either not known or are poorly-defined. Current design principles are based on empirically-derived guidelines that are only useful over a very narrow range of feedstock properties. The work from this task will allow biorefinery designers and operators will be able to design high-temperature unit operations/processes that are flexible and responsive to natural and market feedstock variability, while maximizing productivity.

Outcome: A validated, multiscale experimental and computational framework allowing biorefinery designers/operators to maximize productivity and quality with variable incoming feedstock.

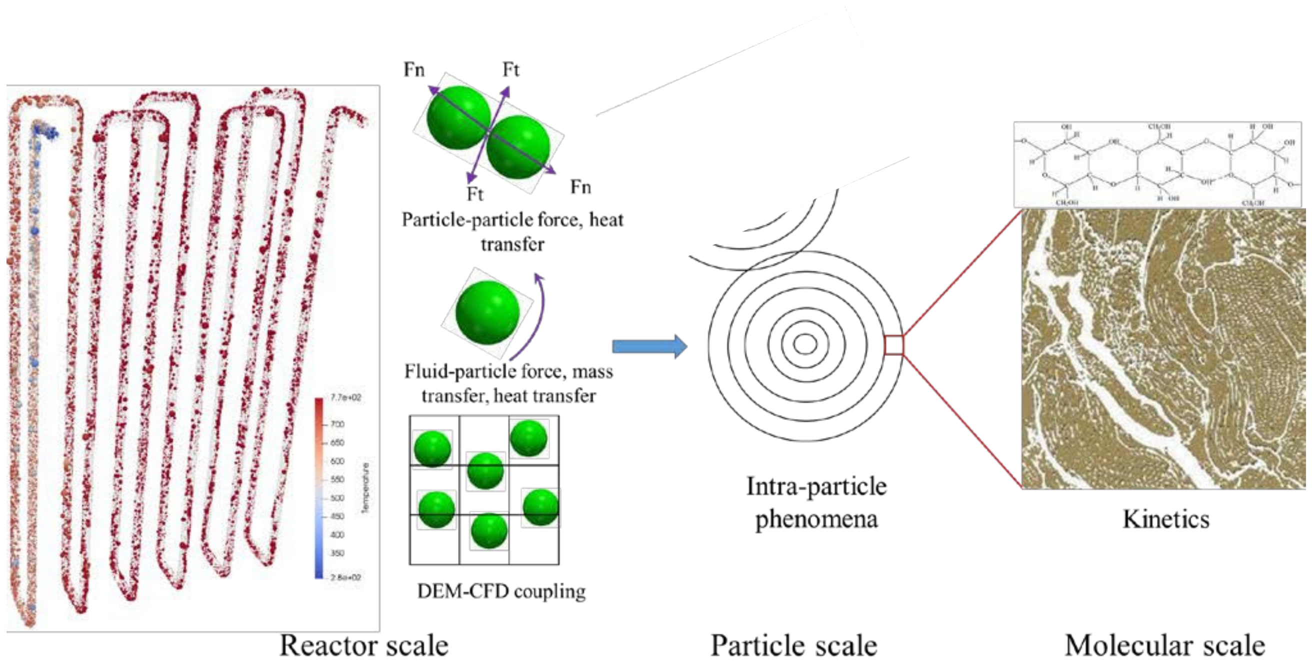
Potential Customers & Outreach Plan:
Potential customers include biorefinery designers and operators. We will communicate new tools to them through publications, presentations, and IAB engagement.



A multiscale approach for biomass pyrolysis

Tools

Implemented a multiscale approach integrating reactor model, particle model and detailed biomass pyrolysis kinetics



Description
- Developed a reduced order particle scale model suitable for large-scale simulation
- A detailed biomass pyrolysis model was coupled to particle scale model
- The multiscale approach model was implemented and validated in the open-source CFD suite MFiX

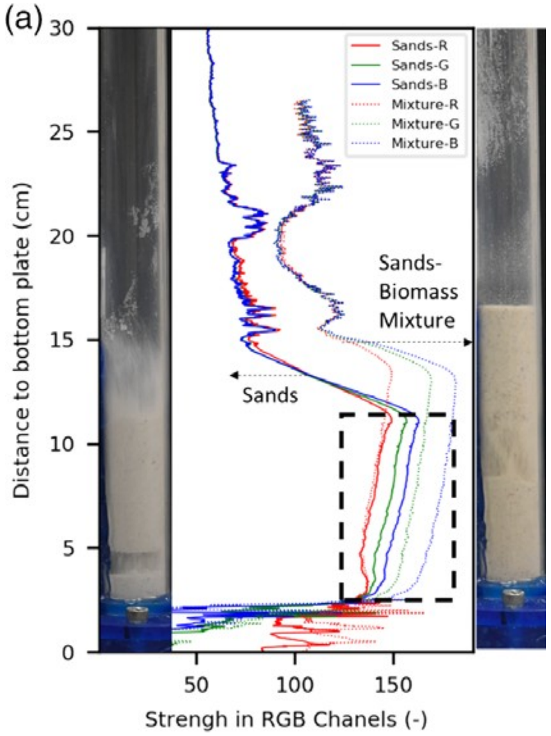
Value of new tool
- The tool can correctly simulate the effect of intraparticle transport phenomena on conversion and product distribution
- This novel multi-scale approach provides an efficient tool for biomass pyrolysis reactors design, optimization and scale-up.

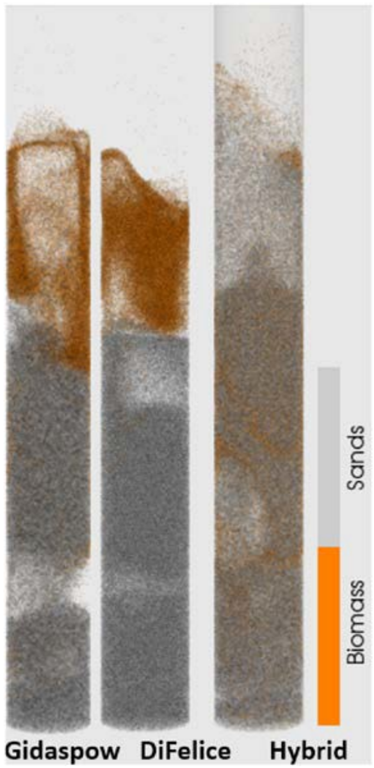
Potential Customers & Outreach Plan
- Biomass pyrolysis reactor designers, operators
- Module freely available for the public in open source MFIX Suite

Hybrid gas-sand-biomass interaction model accurately captures the mixing of sand & biomass

Knowledge

A combined experimental and numerical investigation of biomass and sand co-fluidization





Current Knowledge Gap

- The complex interaction between gas-sand-biomass is not well understood but is of crucial importance to efficient pyrolysis reactor performance
- Variability in feedstock shapes, sizes, and densities creates numerous challenges to stable operation of fluidized bed reactors

Achievement

- Analyzed the sand–biomass mixing using image analysis of high-speed videos and compared to MFiX CFD pyrolysis reactor simulations
- Proposed a novel hybrid drag model captures the mixing of sand-biomass

Relevance

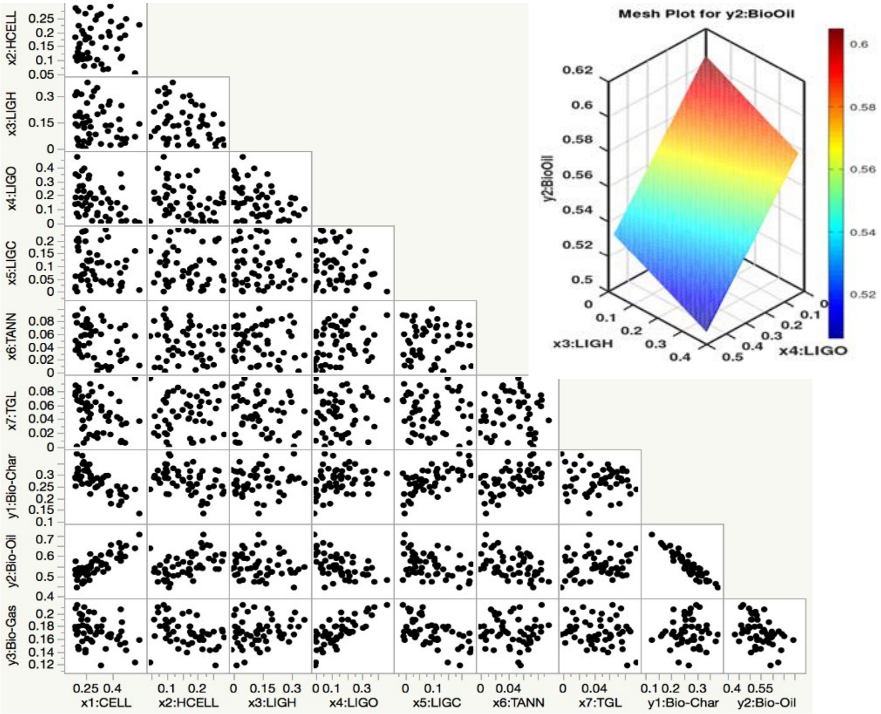
- The complex gas-sand-biomass interaction is understood and explained using MFiX simulations with this novel drag model
- The mixing of sand with various feedstocks can be efficiently investigated with computer simulations using MFiX software and the novel drag model validated in this coupled experiment-simulation research

"Experimental and numerical investigation of sands and Geldart A biomass co-fluidization", Liqiang Lu, Jia Yu, Xi Gao, Yupeng Xu, Mehrdad Shahnam, William A. Rogers, AIChE Journal, https://doi.org/10.1002/aic.16969

Assessing the sensitivity of pyrolysis products to feedstock composition

Knowledge

Global sensitivity analysis determined that the yield of bio-oil is correlated to oxygen-rich lignin



Current Knowledge Gap

- Lignocellulosic biomass is primarily composed of polysaccharidic cellulose, hemicellulose and polyaromatic lignin. However, the influence of these compositions on pyrolysis products is not well understood
- Detailed pyrolysis kinetics mechanism is missing

Achievement

- Implemented a validated detailed pyrolysis kinetics mechanism
- Sensitivity of pyrolysis products to feedstock compositions was investigated by performing a simulation campaign based on statistical design of experiments principles utilizing MFiX-Nodeworks toolset

Relevance

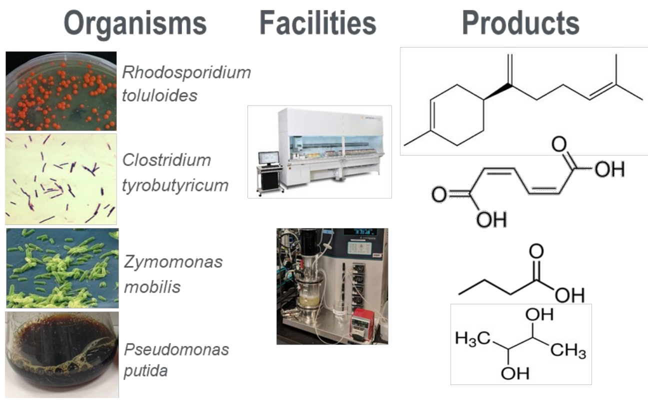
- The complex influence of biomass compositions on pyrolysis products is understood and explained
- The insight gained from this study can be utilized in re-allocating adequate resources to reduce the uncertainties associated with the reaction kinetics of the most influential species

Low Temperature Conversion Task

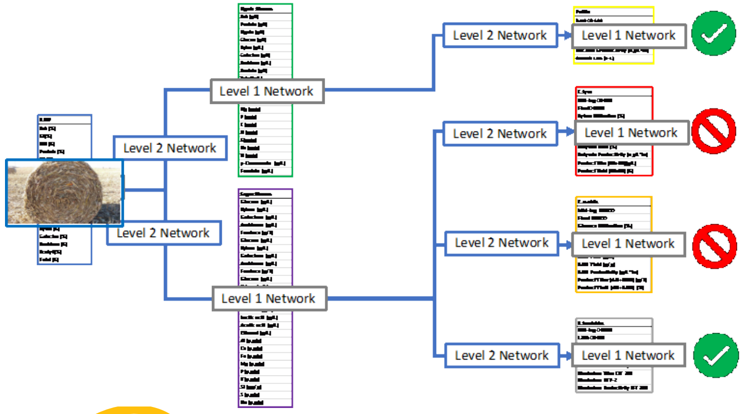
Objective: Determine the effects of biomass feedstock variability on the low-temperature conversion process chain (both sugar and lignin pathways) and develop tools to mitigate the risks posed by this variability.

Impact: The interdisciplinary research team in this Task is uncovering knowledge and developing tools that minimize the impacts of feedstock and process variability. As a result, the sequential cascade of low-temperature processes can intelligently operate by understanding critical attributes of materials passed downstream and by adjusting process parameters that allow for tolerance of upstream complications.

Outcome: Knowledge and tools that mitigate the risks posed by feedstock variability on the performance of low-temperature conversion processes – minimizing variability upstream via first-principles understanding of CMAs that facilitates performance predictability for future low-temperature processes with changes to CPPs downstream .



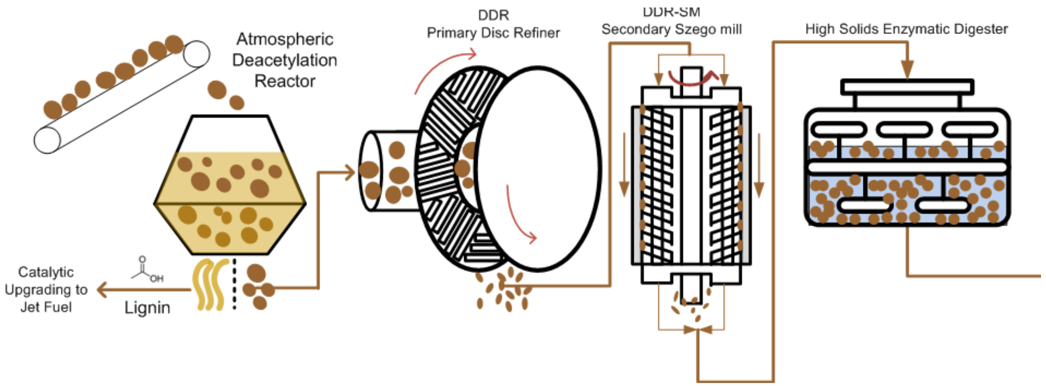
Potential Customers & Outreach Plan: We will produce a robust, validated predictive model for the effects of feedstock and process variability on biocatalyst performance. The model (and the approach) will be of interest to the biomanufacturing industry. We will publicize this work in peer-reviewed journal articles and will identify industry stakeholders (starting with the IAB) to communicate with directly.



Standardized deconstruction conditions produce suboptimal results for recalcitrant anatomical fractions of corn stover

Knowledge

Leaves and husks of corn stover are more readily deconstructed as compared to stalks, and knowledge of differences between anatomical fractions will drive separation economics and optimized processes.



Current Knowledge Gap

- The systematic deconstruction of anatomical fractions of corn stover had never been approached with standardized conditions and sample characterization methods

Achievement

- Three distinct anatomical fractions of corn stover (cobs, husks and leaves, and stalks) were deconstructed by standard conditions with differences in sugar and lignin streams exhaustively characterized and compared to parent materials containing all fractions in proportion.

Relevance

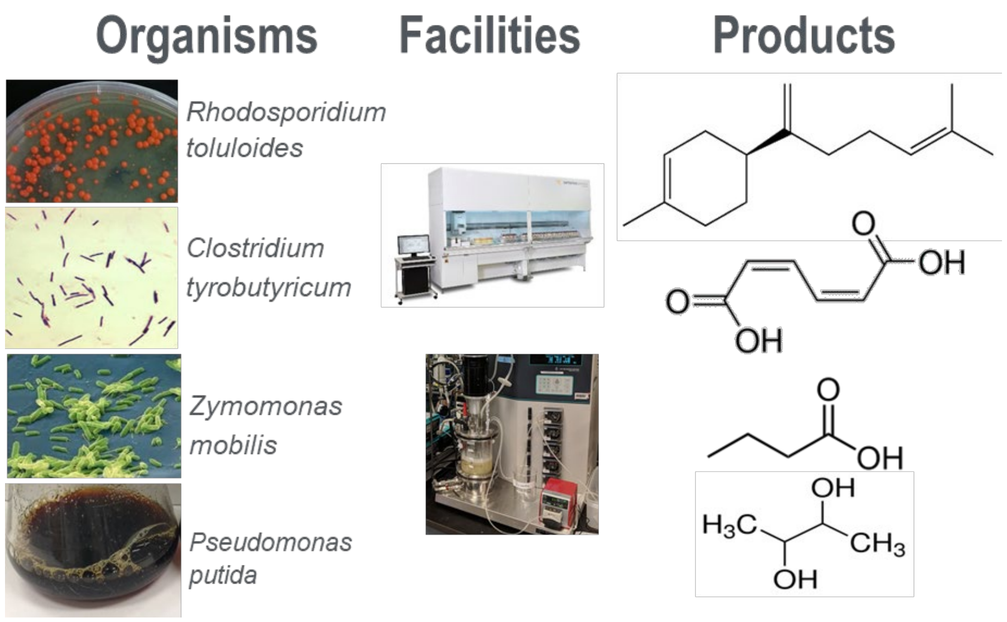
- For the successful use of lignocellulosic materials in biocatalytic conversion, harvesting and deconstruction methods must be co-optimized for development of economically viable processes.
- This work underscores the recalcitrant nature of the bulk of corn stover materials and serves as an example of where the development of standardized methods for bulk material could prove limiting as harvesting methods advance.

Feedstock variability influences titers, rates, and yields of bioconversion processes

Knowledge

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Variability in the quality of raw corn stover materials impacted the titers, rates, and yields of conversion of sugar and lignin streams to bioproducts by a wide array of microorganisms.



Current Knowledge Gap

- Public data regarding the impact of feedstock variability on fermentation organism performance using sugar and lignin streams derived from DMR pretreated biomass

Achievement

- Significant changes (> 15% level) in biocatalytic productivity and substrate utilization were uncovered for feedstocks of varying quality.
- Strikingly, conversion performance was impacted for both the sugar- and lignin-converting organisms, with differential process effects.

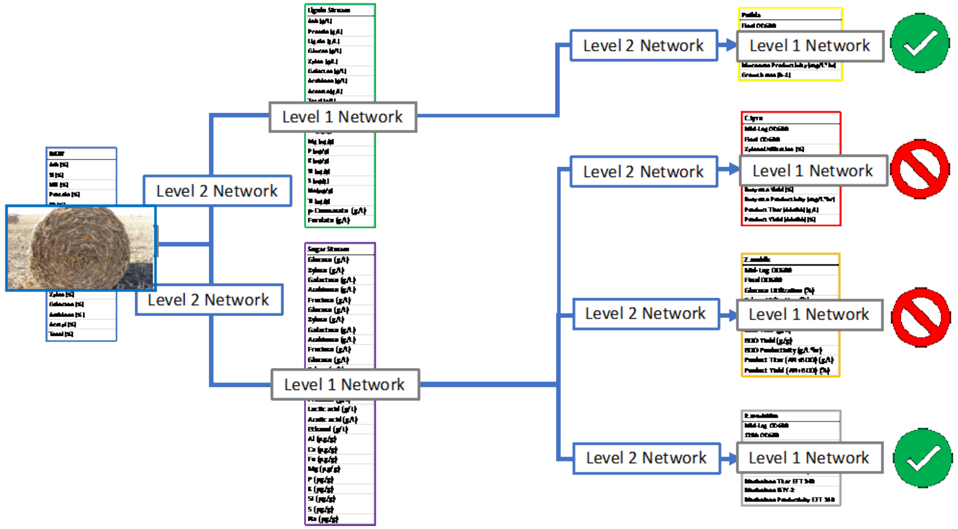
Relevance

- 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 multiple streams arising from DMR pretreatment.
- Previously, with limited data, biorefineries would be forced to accept the performance risk of varying feedstocks or invest substantially to generate scientific data and understanding that are not shared publicly.
- These results will allow the FCIC to develop tools to mitigate the risks posed by this variability.

Tiered interaction networks to optimize bioconversion processes

Tools

Identifying the metabolic basis for the impact of feedstock stream attributes on conversion efficiency will allow low temperature approaches to adapt to and engineer around feedstock variability.



Description

- Causal interaction networks have been established to assess CMAs across multi-step bioprocesses to understand factors that generally and/or differentially, influence bioconversion efficiency.

Value of new tool

- Understanding of why organisms used in low temperature conversion of sugar and lignin streams from corn stover feedstocks are impacted differentially by material attributes
- Combining performance data with metabolic information results in first-principles understanding and *actionable* results, e.g., matching specific biocatalytic agents to feedstocks entering a conversion facility

Potential Customers & Outreach Plan

- The biomanufacturing industry needs tools that identify CMAs for specific feedstock-organism-bioproduct combinations to optimize processes and plant efficiencies. This approach is broadly applicable to any multi-step biocatalytic process.

Materials of Construction Task

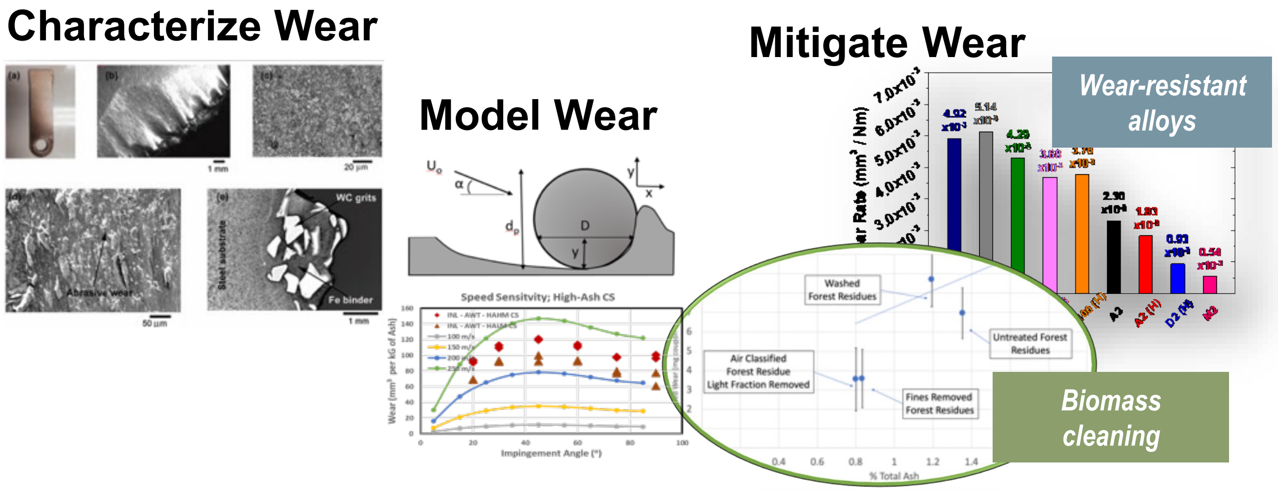
Objective: Using integrated efforts of characterization, modeling, and testing to gain fundamental understanding of failure modes and wear mechanisms, develop analytical tools/models to predict wear and establish material property specifications, select and evaluate candidate mitigations, and share the fundamentals and mitigations with the biomass industry.

Impact: Current approaches use equipment and materials designed for non-biomass feedstocks. The knowledge and tools developed here will enable rapid design and selection of materials that resist wear and maintain structural integrity, resulting in sustainable performance and improved product quality. The science-based approach avoids the time and expense associated with trial-and-error methods.

Outcome: Develop knowledge and tools to understand how to measure, predict, and mitigate wear.

Potential Customers & Outreach Plan:
Potential customers include plant engineering firms and operators, equipment manufacturers, and component suppliers.

We will communicate new tools to them through publications, presentations, review meetings, and FOA teaming.



Correlating extrinsic and intrinsic inorganic compounds with preprocessing tool wear

Knowledge

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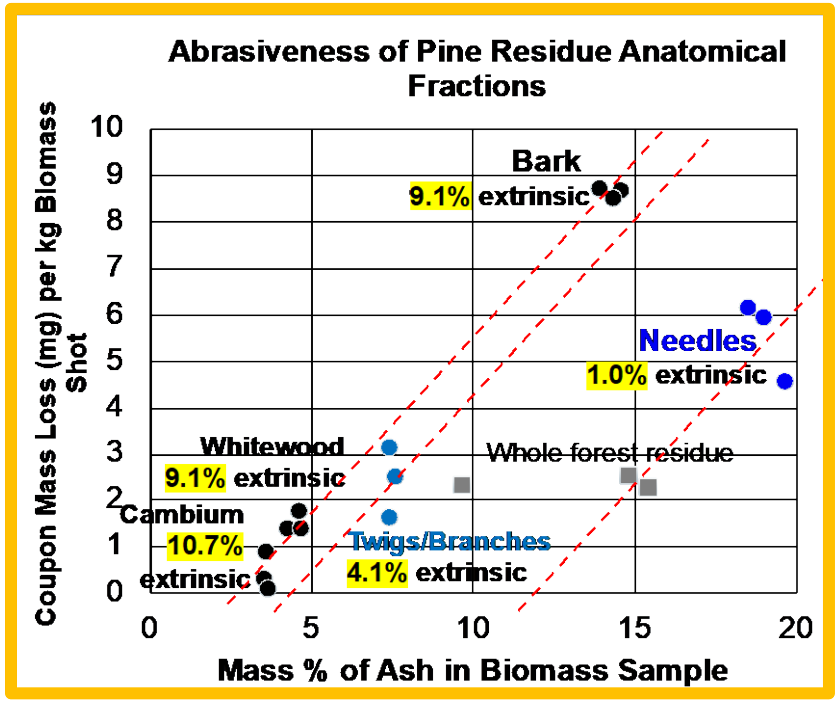
Developed new composition-preserving methods for extracting & characterizing biomass inorganics and identified correlations with tool wear



Composition-Preserving Extraction and Characterization of Biomass Extrinsic and Intrinsic Inorganic Compounds, *ACS Sustainable Chemistry & Engineering* (2020) 8, 1599-1610, https://dx.doi.org/10.1021/acssuschemeng.9b06429

Current Knowledge Gap

The inorganic compounds of biomass feedstock are suspected to be the major cause for equipment wear in biomass processing. Conventionally, the inorganic content of biomass is determined by measuring the residue weight after combustion, called "ash," which includes both noncombustible inorganics and new compounds formed by oxidation and decomposition.

Achievement

We developed composition-preserving methods to extract and characterize biomass inorganic compounds to allow a better understanding of their correlations to the preprocessing tool wear. We concluded that both intrinsic and extrinsic inorganic compounds contribute to tool wear, but the extrinsic minerals are much more abrasive than the intrinsic inorganic compounds.

Relevance

These results will inform TEA models, which can determine tradeoffs between tool material wear and cost, as well as inform harvest practices, which have the possibility to increase or decrease inorganics.

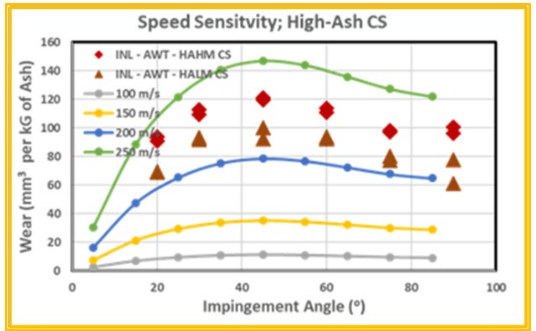
Modeling wear as functions of material attributes and process parameters

Knowledge

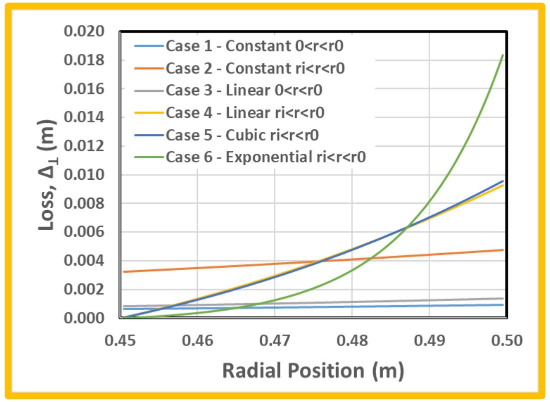
Developed erosive wear model that relates feedstock attributes (MAs), component attributes (MAs), and process parameters (PPs) to critical quality performance attributes (wear and component shape)

$$\frac{\Delta Q}{m_p} = C_D * \frac{\rho_p^{\left(\frac{1}{4b}\right)} * (U_0 \sin\alpha)^{\left(2+\frac{1}{2b}\right)}}{\eta^{\left(\frac{3}{4b}\right)} \varepsilon_f^{\left(\frac{1}{b}\right)} H^{\left(1+\frac{1}{4b}\right)}} + C_C(1+f) * (1-\exp(-200\alpha^2)) \frac{\rho_p^{\frac{1-f}{2}} d_p^{(1-f)}}{\eta^{\frac{1-f}{2}} H^{\frac{1-f}{2}} R^{(1-f)}} [U_0^{(3-f)} \cos^2(\alpha) \sin^{(1-f)}(\alpha)]$$

Ben-Ami erosion wear model



Predicted & Measured Simulation Wear



Predicted Hammer Wear

Current Knowledge Gap

Biomass size reduction equipment experience wear issues that significantly impact biorefinery economics. The effects of both feedstock and materials of construction properties on equipment wear need to be identified and quantified.

Achievement

We developed predictive models of erosive wear, guided by simulation studies and material characterization of worn components. Ash content, impingement angle, and radial position were correlated with erosive wear. We validated the simulation studies with excellent agreement between the predictive model and experimental wear data.

Guided by the predictive wear model, sensitivity studies were performed to determine the impact of critical component material properties (hardness, toughness, and fatigue ductility) on predicted wear. Increasing the value these properties reduces wear, so we began evaluating novel solutions involving boride coatings.

Relevance

Results provide the ability to screen effects of feedstock attributes and process parameters on wear and performance, enabling the development of material property and feedstock specifications. This will inform TEA models and allow biorefineries to choose feedstock attributes and size reduction materials of construction.

Crosscutting Analyses Task

Objective: Quantify and communicate industrially relevant, system-level cost and environmental impacts for the discoveries and innovations of the FCIC through well-documented Case Studies to quantify how feedstock variability affects underlying economics and sustainability metrics through the entire value chain, from feedstock production through preprocessing and conversion

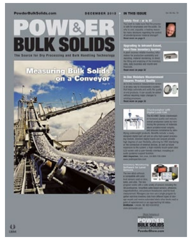
Impact: The Case Studies will allow industry stakeholders to quickly understand the TEA and LCA implications of feedstock variability, and will better appreciate the knowledge and tools developed by FCIC researchers to address this variability

Outcome: Cost-benefit TEA and LCA Case Studies that valorize the impacts of feedstock variability on biorefinery yields, economics, and environmental sustainability to aid engineers and equipment manufacturers conducting feasibility studies of proposed equipment and process design modifications

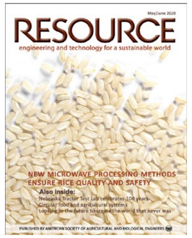
Potential Customers & Outreach Plan:

- Customers are bioenergy industry stakeholders across the value chain
- Engaging FCIC IAB for feedback on case study formulation, approach, assumptions
- 1-pagers highlighting highest impact case studies on FCIC website
- Conference presentations and associated trade journals

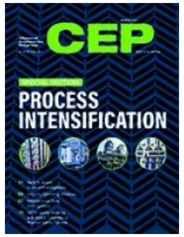
INTERNATIONAL POWDER & BULK SOLIDS CONFERENCE & EXHIBITION



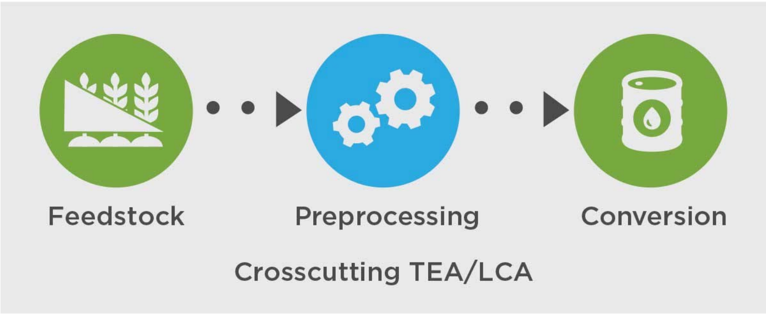
ASABE

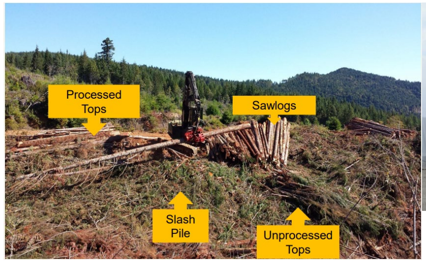


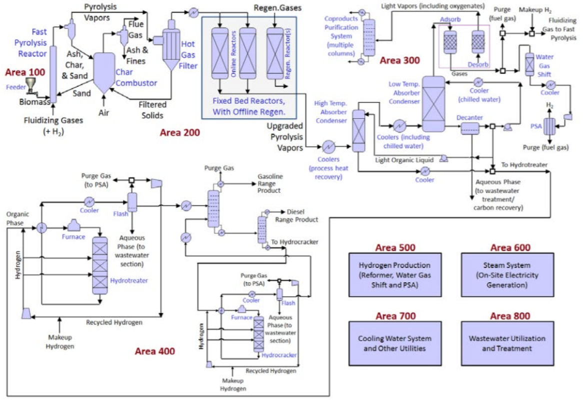
AIChE



Bioenergy Value Chain







MFSP impacts predicted from fast pyrolysis product yields based on particle-level modeling

Knowledge Gap

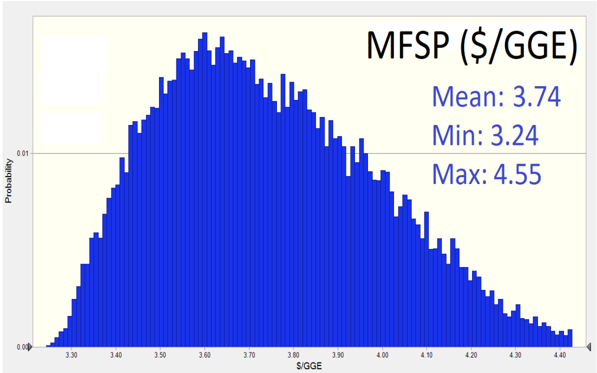
- TEA impacts of feedstock material attributes and process parameters associated with fast pyrolysis are not well-understood

Achievement

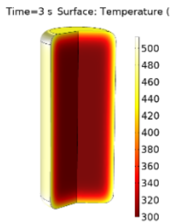
- Particle-scale model, validated from literature, was used in combination with multiple linear regression models to develop high-level correlations of each varied parameter linked to fast pyrolysis (FP) oil yield and char yield.
- CFP fuel carbon efficiency (1) and char yield (2) were correlated with MFSP from multiple runs of Aspen model. % change in FP-oil yield and char yield predicted by particle modeling correlations were linked with % changes in (1) and (2), and then to the MFSP.
- Distributions of varied parameters were used in Monte Carlo simulations to understand their impacts on MFSP

Relevance

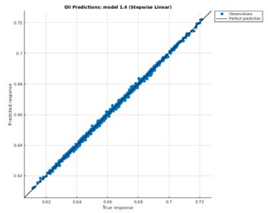
- Correlations can capture impacts of variation in feedstock attributes on the MFSP
- Increase in mineral matter was shown to have the biggest impact, predominantly due to reduced FP oil yield.
- Current correlations are for fast pyrolysis yields; assumes direct correlation between FP oil and CFP fuel yields; future work will establish more detailed linkage; current predictions are directionally correct and provide insights



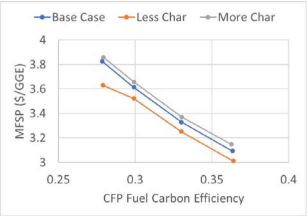
Varied Parameters	
FP Material Attributes (**MAs**)	• mineral matter composition • moisture content • particle diameter • extractives content
FP Process Parameters (**PPs**)	• reactor temperature



Validated Particle-Scale Model (Task 6.3) →



Multiple Linear Regression Models (Task 6.3) →



Link with MFSP from CFP TEA models (Task 8.3) → **MFSP**

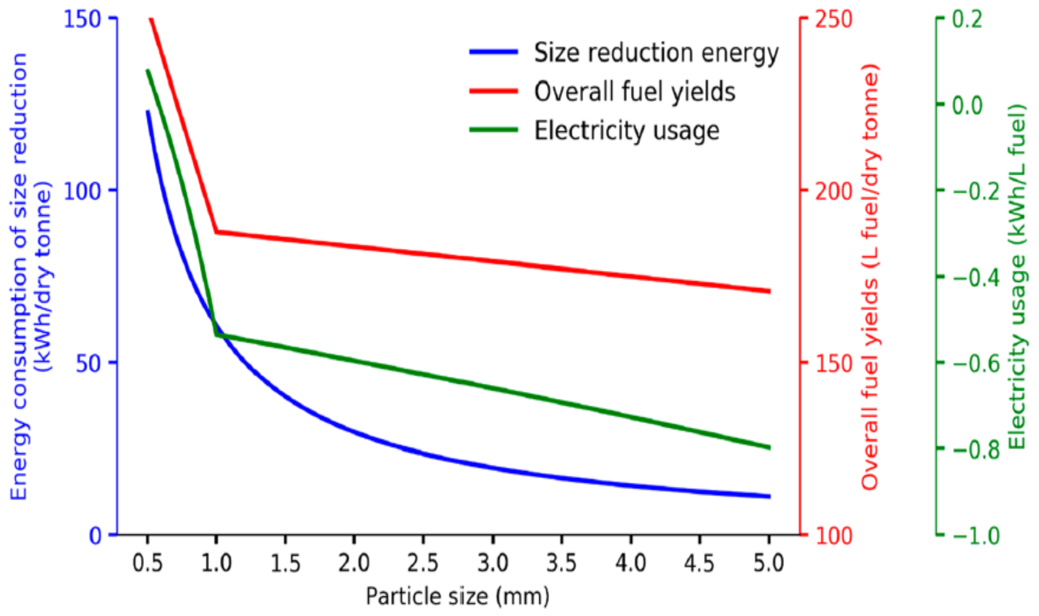
MFSP: Minimum Fuel Selling Price; **FP**: Fast Pyrolysis; **CFP**: Catalytic Fast Pyrolysis; **TEA**: Techno-Economic Analysis

Contributors: Pecha, Crowley, Ciesielski, Dutta, Wiatrowski, Carpenter
Key Collaborations: CCPC and Thermochemical Platform Analysis (2.1.0.302)

Addressing unit operation-level causal effects with dynamic LCA

Knowledge

Dynamic LCA addresses the impacts of feedstock variability on system sustainability focusing on unit operational causal effects.



Current Knowledge Gap

- What are the causal effects between feedstock CMAs, CQAs, and CPPs across key unit operations of the fast pyrolysis conversion platform?
- How do the CMAs, CPPs, and CQAs of key unit operations affect system sustainability?

Achievement

- Demonstrated application of a dynamic LCA framework to address system-wide sustainability impacts of CMAs, CPPs, and CQAs across the supply chain and unit operations.
- Developed quantitative relationships between feedstock properties (particle size and moisture content) and key unit operations (preprocessing energy requirement, pyrolysis yields, and overall electricity usage/credits, etc.) that affect system-level sustainability.

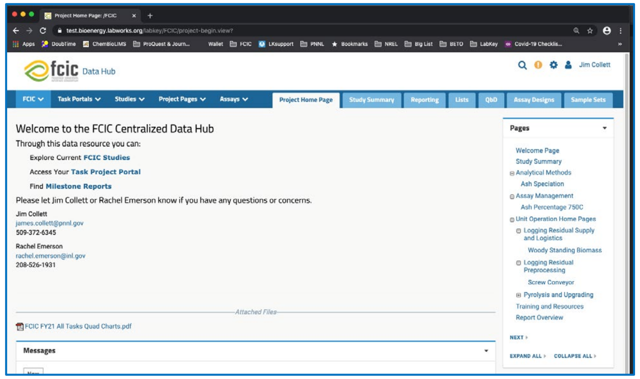
Relevance

- Dynamic LCA can improve our understanding of life cycle implications of key CMAs and CPPs when relevant data is available.
- Dynamic LCA can address sustainability impacts of novel technologies such as feedstock fractionation, preprocessing, and conversion technologies.

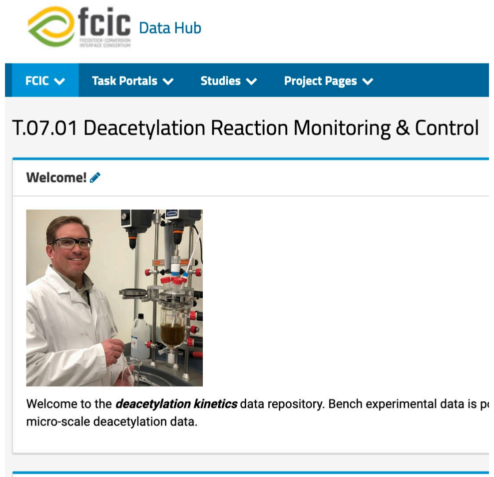
"Dynamic Life-Cycle Analysis of Fast Pyrolysis Biorefineries: Impacts of Feedstock Moisture Content and Particle Size" Longwen Ou and Hao Cai, *ACS Sustainable Chemistry & Engineering* 8(16): 6211-21. https://pubs.acs.org/doi/10.1021/acssuschemeng.9b06836

Data Integration and QbD Task

Objective: Task 4 is building database tools for integrating CMAs, CPPs, CQAs and experimental data from across FCIC the within the LabKey Data Hub hosted on the AWS cloud. We are providing a collaborative computational environment for hypothesis development, experimental and modeling workflow management, integration of datasets and metadata, and deliverables sharing between FCIC subtasks and a portal for public access to FCIC results, data, and software.



Impact: This task provides the necessary infrastructure for FCIC researchers to store and integrate their experimental results according to FAIR guidelines and is enabling easier collaborations among tasks.



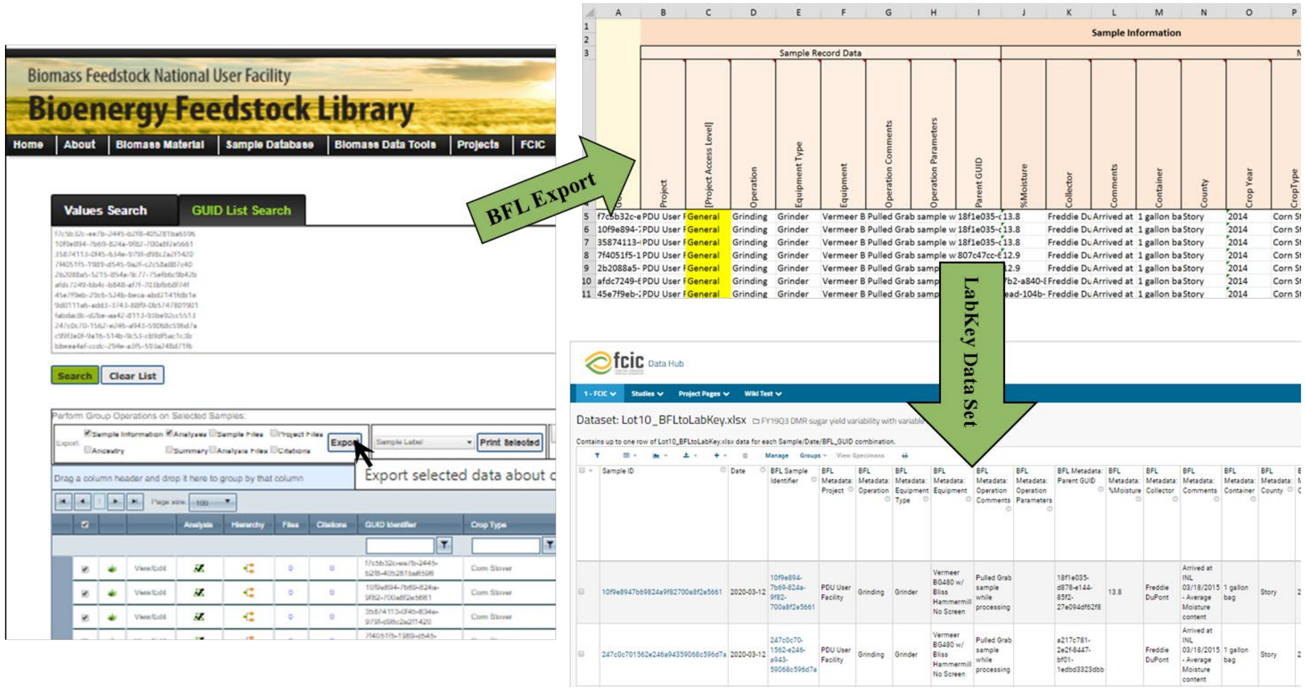
Outcomes:

- A web-based platform accessible to all FCIC researchers and stakeholders to provide data and knowledge on the effects of feedstock variability
- A means to harmonize data across the FCIC; and tools to facilitate sharing of Case Study results, including Case Study experimental datasets and cost analysis results.

LabKey/BFL increased interoperability

Tools

Creation of LabKey Datasets directly from Bioenergy Feedstock Library (BFL) exports



Description

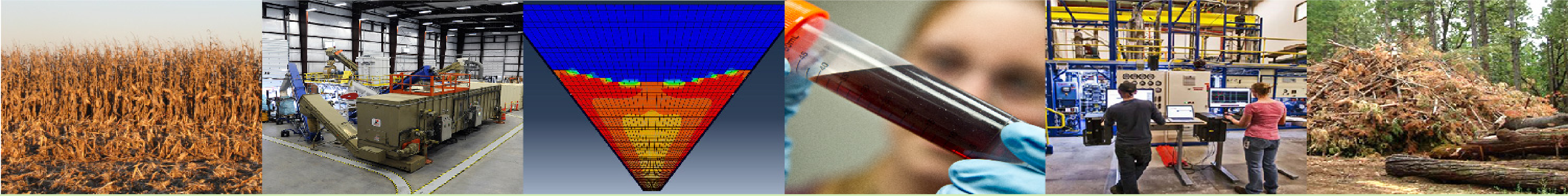
A Python based script was developed to directly create Study data sets (tabular representations of the data collected for samples within a study) from data exported from the Bioenergy Feedstock Library (BFL)

Value of new tool

The tool reduces the need to manually create redundant data structures between the two systems and represents an additional method to establish interoperability between the BFL and LabKey.

Potential Customers & Outreach Plan

INL researchers can more easily import samples and data directly into LabKey that are being tracked in the BFL database system.



Industry Advisory Board

FCIC
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

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Foster Agblevor

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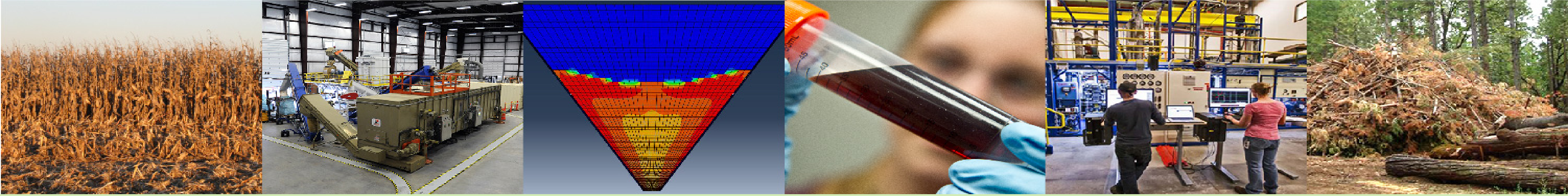

DFOs

DFO – Working with Industry

A 2017 Directed Funding Opportunity (DFO) resulted in six funded projects – 30% cost-share

Wonderful Company/NREL/INL

- Feeding issues associated with small-scale gasification systems

Idaho Forest Products/INL

- Advanced processing control systems – scope under revision

Fulcrum Bioenergy/INL

- Densification of MSW feedstock streams

Forest Concepts/ORNL/INL

- Wear issues associated with comminution technologies

Jenike & Johansen/LANL

- On-line acoustic water measurement and control

Red Rocks Biofuels/INL/NREL

- Scope currently under revision

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FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Feedstock-Conversion Interface Consortium (FCIC) Directed Funding Opportunity (DFO)

Section 1 – Description

FCIC Publications

FCIC Researchers are publicizing the details of their work in multiple ways – primarily in FY20 with peer-reviewed publications

Publication Type	FY20 Count
Journal Articles	29
Presentations	18
Book Chapters	1
Posters	1
Fact Sheet	1

https://www.energy.gov/eere/bioenergy/fcic-publications

FCIC Contact Information

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