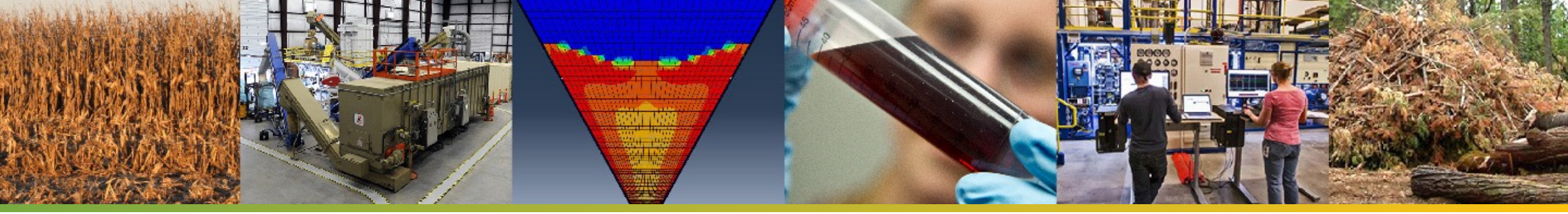

DOE Bioenergy Technologies Office (BETO)
2023 Project Peer Review

FCIC Task 5 – Preprocessing

April 6, 2023
Feedstock-Conversion Interface Consortium (FCIC)

Jordan Klinger
Idaho National Laboratory (INL)

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM
U.S. DEPARTMENT OF ENERGY

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FCIC Task Organization

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

Task 2: Feedstock Variability

Task 5: Preprocessing

Task 6: High-Temperature Conversion

Task 1: Materials of Construction

Task 7: Low-Temperature Conversion

Task 3: Materials Handling

Enabling Tasks

Task X: Project Management

Task 4: Data Integration

Task 8: TEA/LCA
Task 9: FMEA

Task X: Project Management: Provide scientific leadership and organizational project management

Task 1: Materials of Construction: Specify materials that do not wear or break at unacceptable rates

Task 2: Feedstock Variability: Quantify and understand the sources of biomass resource and feedstock variability

Task 3: Materials Handling: Develop tools that enable continuous, steady, trouble-free feed into reactors

Task 4: Data Integration: Ensure the data generated in the FCIC are curated and stored; FAIR guidelines

Task 5: Preprocessing: Enable well-defined and homogeneous feedstock from variable biomass resources

Tasks 6 & 7: Conversion (High- & Low-Temperature Pathways): Produce intermediates for further processing

Task 8: Crosscutting Analyses (TEA/LCA): Valuation of intermediate streams and quantify variability impact

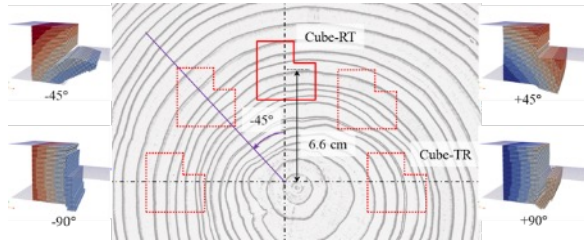
Task 9:Failure Mode & Effects Analysis (FMEA): Standardized approach for assessing attribute criticality

LCA: life cycle analysis; TEA: techno-economic analysis

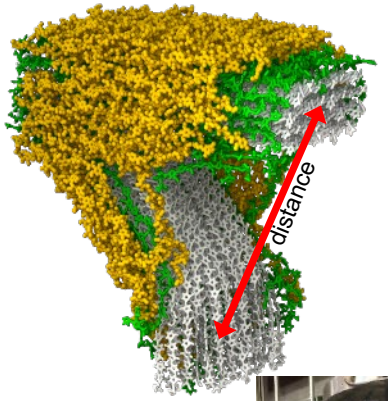
Preprocessing Task

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 subtask meets the objectives of the FCIC by developing transfer functions for comminution, fractionation, deconstruction, and process control that can be utilized by industry to develop new designs for these unit operations that meet critical material attributes (CMAs) for sustainable aviation fuel (SAF).



Outcome: Comminution and fractionation manuals will contain design principles for various working envelopes of CMAs and critical process parameters (CPPs) for corn stover, forest resides, and municipal solid waste (MSW) that reliably produce critical quality attributes (CQAs) necessary for downstream conversion of feedstocks to SAF. Manuals will be made available on the FCIC website and disseminated at trade shows.



Potential Customers & Outreach Plan:

- Direct industry partnerships with JRS, Forest Concepts, and new partners (Andritz and Colorado Milling). Use contacts within INL Biomass Feedstock National User Facility (BFNUF) industrial partnerships.
- Present research at trade shows including ASABE, Powder & Bulk Solids, AIChE.
- 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.

Preprocessing Task

Unit Operation	CMA	CPP	CQA
Comminution	Storage history, growth conditions, moisture, tissue types	Tip speed, screen size, feed rate	Particle Size Distribution (PSD), shape, fines
Fractionation	Moisture, ash, storage history, growth conditions	Air flow, feed rate	Tissue separation
Mesoscale modeling	Biopolymer composition, microstructures, moisture (on other feedstock types including MSW, anatomical fractions)	Comminution method, time, energy, mill speed, feed rate	PSD, shape, fines, bulk density, friction coefficients
Process control	Feedstock types (including MSW), PSD, shape (fines/fluff/stringy), color	Feed rate/residence time, deconstruction reaction severity (chemical loading, temperature)	Flowability, bridging, feeder torque, recalcitrance

Preprocessing Team

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Vicki Thompson, Ph.D.

Neal Yancey

Peter Ciesielski, Ph.D.

Xiaowen Chen, Ph.D.

Meagan Crowley, Ph.D.

Yudong Li, Ph.D.

Richard Elander, Ph.D. (previous member)

Kenneth Sale, Ph.D.

Approach

Technical Approach

Use multiscale experimental and modeling techniques to understand how material attributes and strength properties translate to comminution performance, and how critical attributes for conversion may be changed across preprocessing methods.

Challenges

- Complex breakage mechanisms; different mechanics among different materials.
- Comminution performance is sensitive to both material properties and mill conditions and configuration.

Metrics

- **Go/No-Go decision gate:** Evaluate fidelity of experiment-informed numerical modeling approaches for corn stalk bending properties and breakage in a primary size reduction mill.
- **Economic metrics:** Energy consumption during size reduction; loss of material as fines.
- **Technical metrics:** Particle size and morphological distributions, fraction of constituents in material mixtures, fiber maceration.

Approach

Risks/Mitigation Strategies

- Highly variable nature of biomass and waste; high degree of repetition and multiscale experimentation.
- Fidelity of physical fracture models; experiment-guided simulations to refine particle models and properties.
- Computational cost for at-scale simulations; reduced-order or reduced-throughput simulations to mitigate.

Communication/Collaboration

- WBS 1.2.1.2: Biomass Size Reduction, Drying, and Densification (INL)
- WBS 1.2.1.7: Municipal Solid waste Decontamination (INL)
- WBS 2.5.1.702: Improvement with Rotary Shear Size Reduction (NREL, INL, CCPC, Forest Concepts)

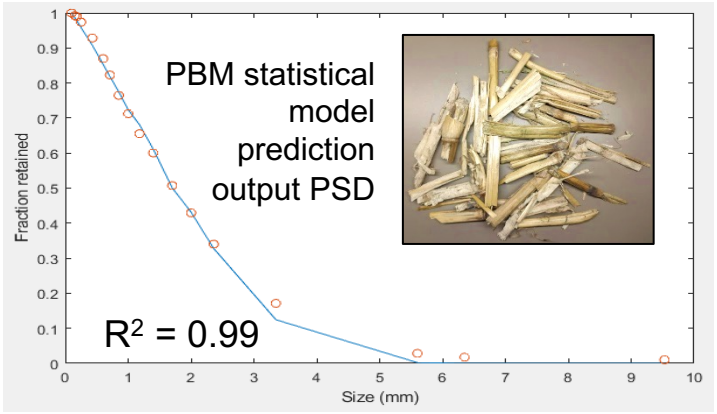
Diversity, Equity, and Inclusion

- Bioenergy- and STEM-focused outreach to traditionally underrepresented high schools.
  - Job shadow events, internships and team opportunities, visits and tours, lectures and demonstrations.
- Open-access tools and documents.

Pilot-Scale Milling Prediction Model Tools

Tools

Developed experiment-informed statistical and physical pilot-scale knife milling models



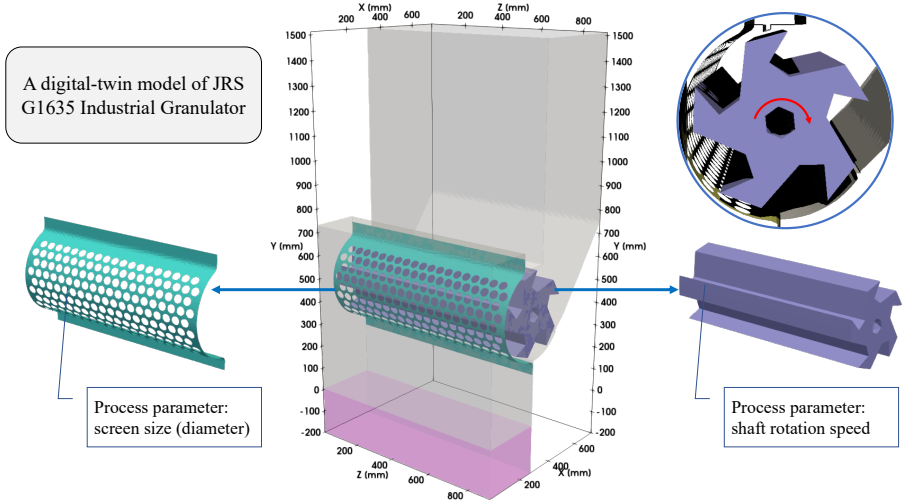
Description

- Developed a pilot-scale knife milling population balance method (PBM) statistical model and discrete element method (DEM) physics model for predicting corn stover deconstruction.

Value of New Tool

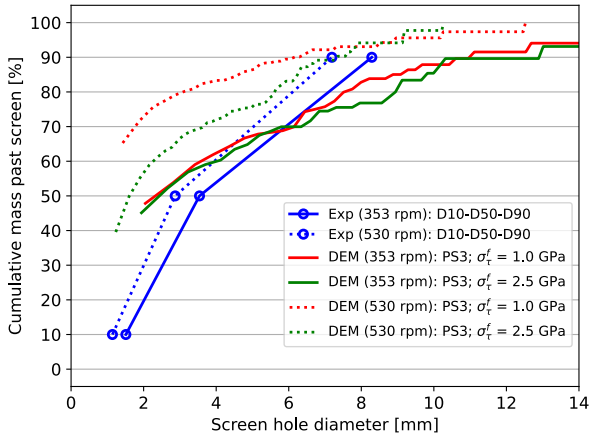
- PBM model allows rapid assessment of output PSD based on feed PSD without requiring expensive experimentation at pilot scale.
- DEM model allows exploring the impacts of specific CPPs and CMAs on output PSD and throughput rate without resorting to testing at scale.

A digital-twin model of JRS G1635 Industrial Granulator

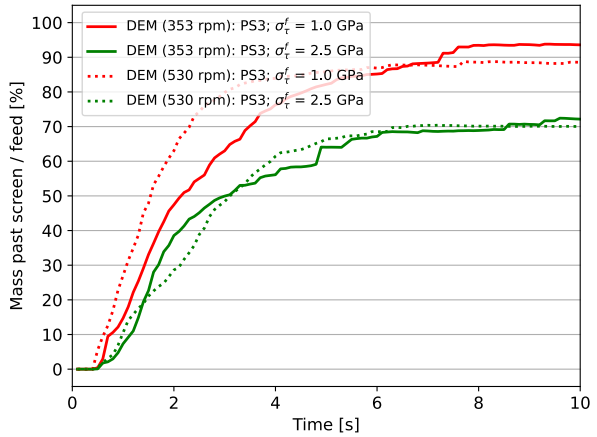


DEM model allows parametric study on:

- Screen size (CPP)
- Shaft rpm (CPP)
- Feed particle size (CMA)
- Feed particle strength (CMA)
- And more…



DEM model prediction output PSD



DEM model prediction of throughout

Biomechanical Properties of Corn Stover

Knowledge

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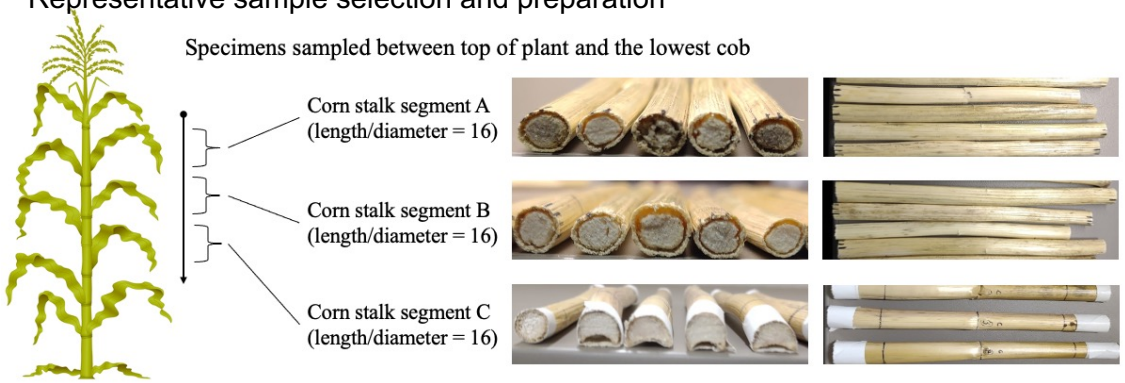
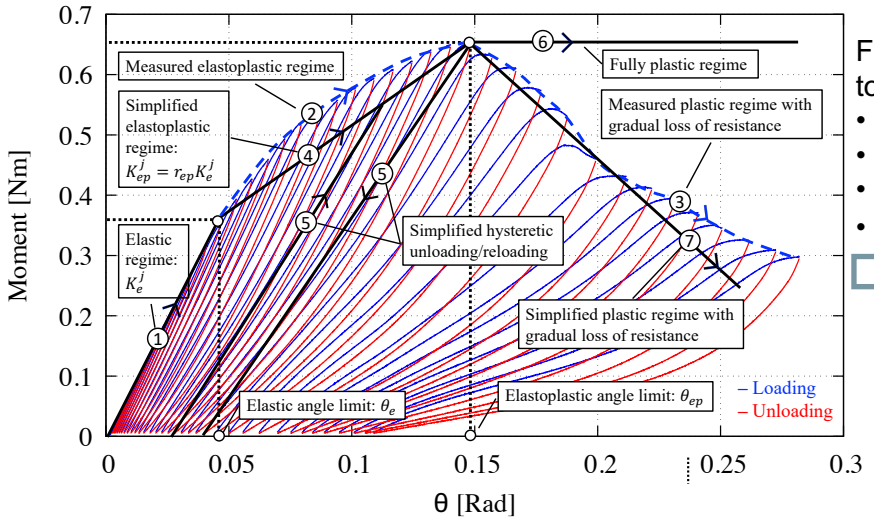
Enhanced understanding of the elastoplastic flexural behavior of corn stalks

Representative sample selection and preparation





From custom 3-point test to summarized CMA data:

- Elastic angle limit
- Elastic bending stiffness
- Elastoplastic angle limit
- Plastic ratio.

Current Knowledge Gap

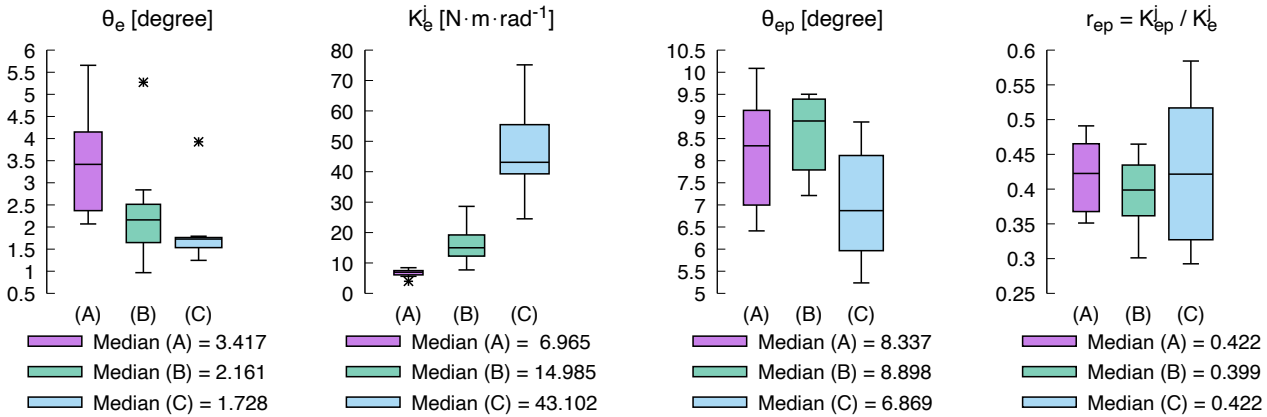
- Lack of sufficient experimental data of flexural behavior of corn stover for developing and validating physics-based biomass comminution models.

Achievement

- Developed a custom three-point cyclic bending-recovery experiment for characterizing the elastoplastic flexural behavior of corn stalks.

Relevance

- Provided CMA data for calibrating DEM corn stalk models in comminution process simulations.
- Provided methodological foundation for developing further sophisticated flexural models for corn stalks and other similar feedstock materials.



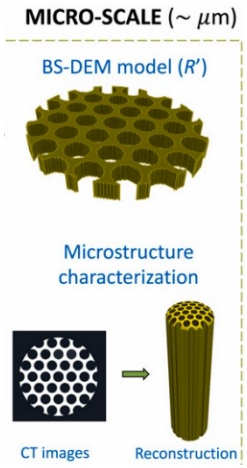
Y. Xia, J. Klinger, T. Bhattacharjee, V. Thomson, "The elastoplastic flexural behavior of corn stalks." *Biosystems Engineering* 216 (2022): 218-228. https://doi.org/10.1016/j.biosystemseng.2022.02.016

Idaho National Laboratory

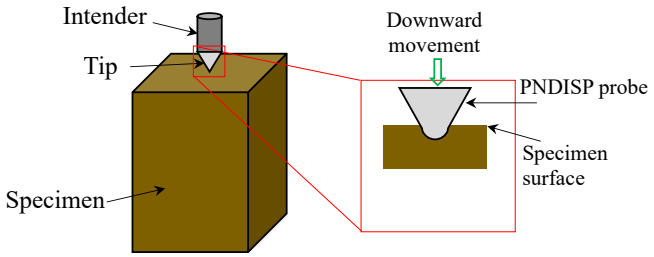
Pine Microstructural & Mechanical Model

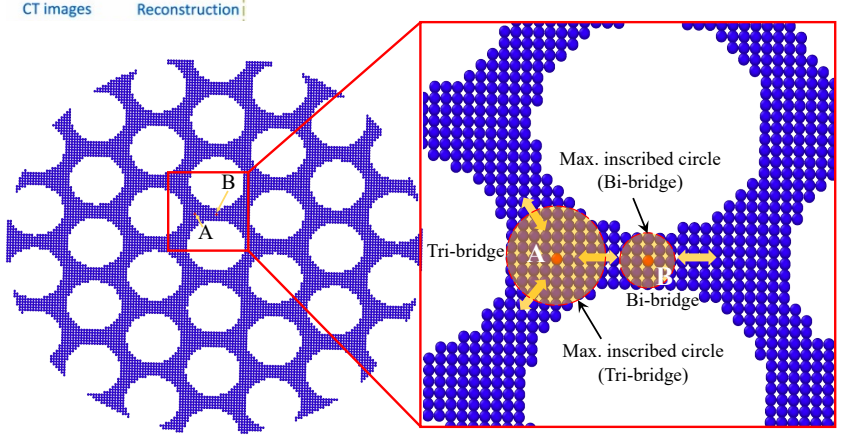
Tools

Developed microindentation experiment, validated pine microstructural mechanical model as part of a multiscale analysis tool



Task 2: Feedstock Variability provided micro-indentation experimental reference and data.





Microstructural DEM model allows parametric study on:

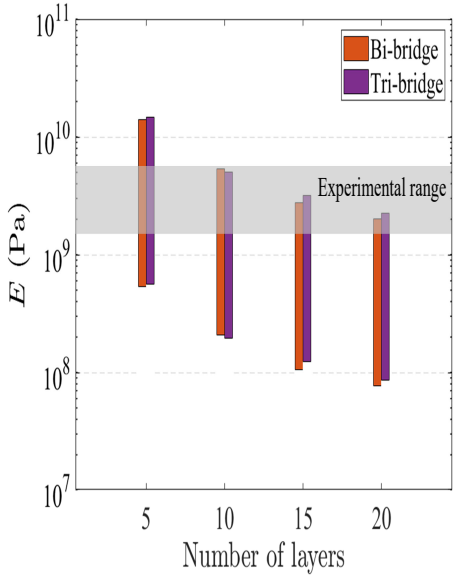
- Loading location (CPP)
- Loading orientation (CPP)
- Material stiffness (CMA)
- Material critical strength (CMA)
- And more…

Description

- Developed a reverse-scaling model for determining microscale DEM model parameters informed by macroscale pine mechanical properties.

Value of new tool

- Open-source to allow lab-to-lab/industry collaborations.
- An intermediate-scale model links mesoscale model (NREL) and macroscale model (INL) in the multiscale model plan.



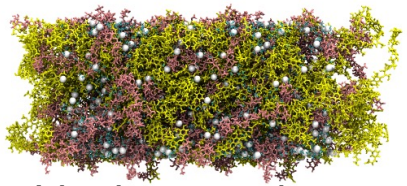
Q. Sun, Q. Chen, **Y. Xia**, F. Chen, J. Klinger, L. Ding, V. Thompson, "Reverse scaling of a bonded-sphere DEM model: Formulation and application to lignocellulosic biomass microstructures." *Powder Technology* 407 (2022): 117797. http://dx.doi.org/10.1016/j.powtec.2022.117797

Polymer Assembly Strength Models

Knowledge

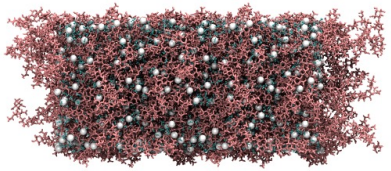
fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM U.S. DEPARTMENT OF ENERGY

Molecular studies of the middle lamella reveal the function of individual biopolymer components

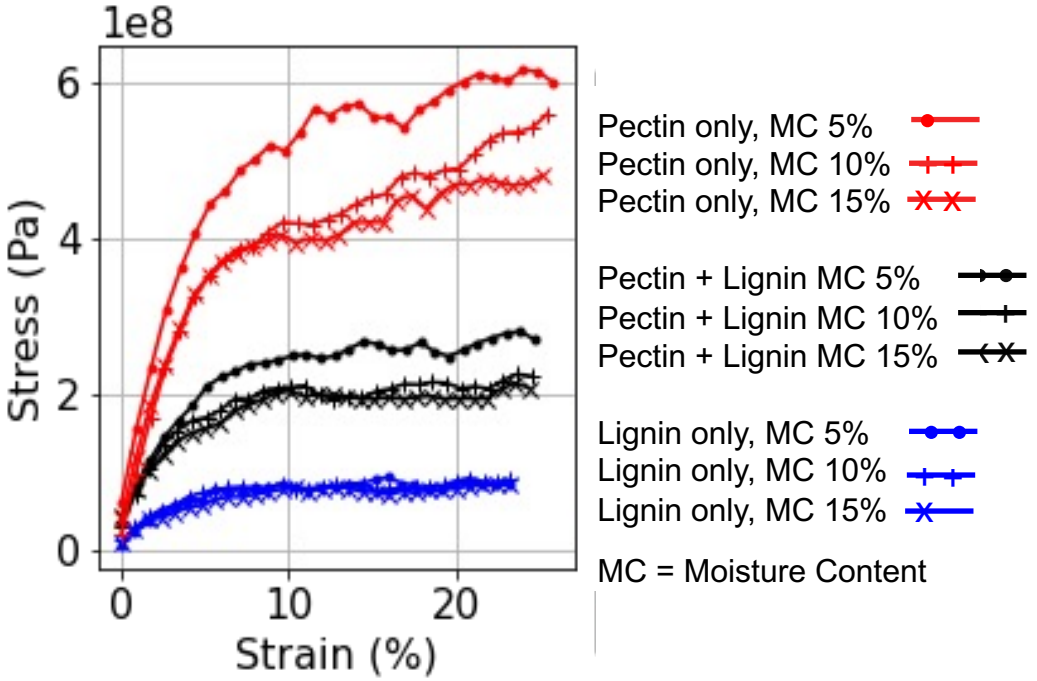


Lignin + pectin

Pure lignin



Pure pectin



Current Knowledge Gap

The middle lamella is a specialized tissue type that adheres adjacent cells and tends to be the primary location of failure during comminution. The function of its unique biopolymer composition is unclear.

Achievement

Molecular models with varying biopolymer composition and moisture content were subjected to tensile tests *in silico*. The results identified:

- **Lignin acts as a plasticizer in the middle lamella.**
- **Assemblies of pectin only are stiff and brittle.**
- **Assemblies of lignin only are soft relative to carbohydrate polymers.**
- **Moisture acts as a plasticizer only if pectin is present.**

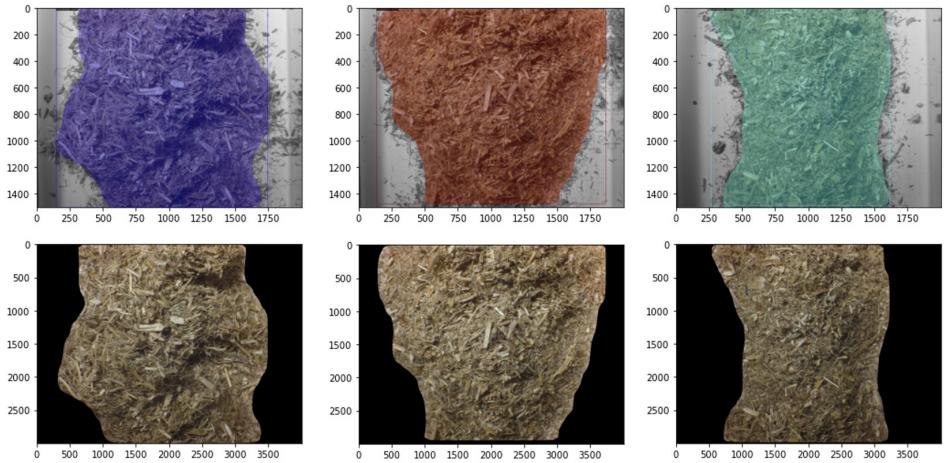
Industry Impact

These observations define a roadmap for chemo-mechanical processing methods to identify the sequence of biopolymer fractionations that minimize mechanical energy input.

Real-Time Feedstock Image Analysis Model

Tools

Automated machine vision technique to detect and quantify corn stover feedstock particle quality in real time



Description

- Generated corn stover image segmentation data set for neural network training.
- Deep neural network model was developed and trained to perform automated biomass segmentation to remove irrelevant background for further prediction of biomass properties.

Value of New Tool

- The developed model is capable of automatically identifying where the corn stover is located in an image and labeling the image for segmentation/background removal.
- The tool will facilitate more accurate feedstock properties prediction in future model development.
- The tool can be easily trained to perform auto-segmentation of different feedstocks with data sets generated for the feedstock.
- This tool can be easily served using a web app to reach a broader customer base due to its easy-to-use feature. A web app called EasyVision is currently under development to serve this tool/model.

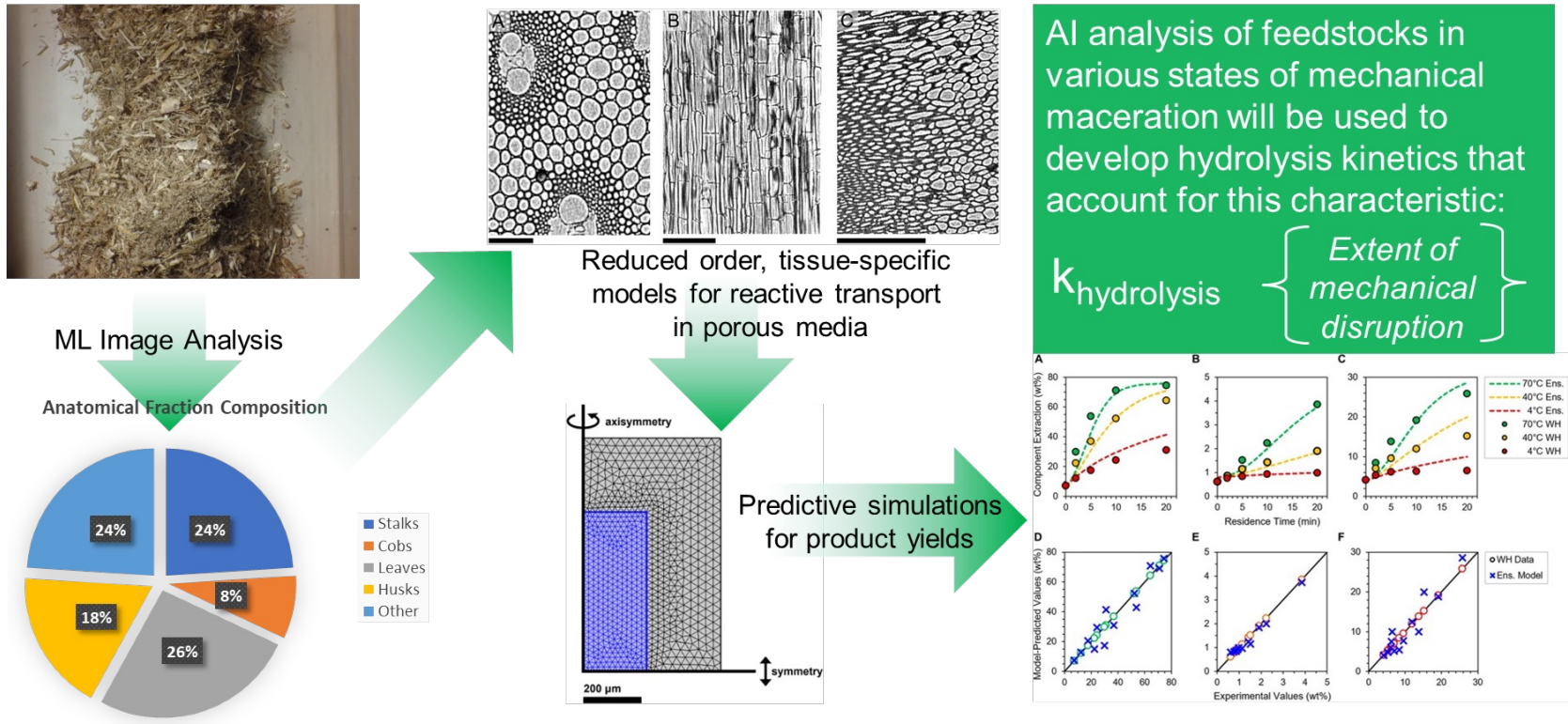
Potential Customers & Outreach Plan

- In FY23, we plan to reach out to companies to form collaboration connections to facilitate the development/deployment of our tool. Such companies may include WipWare and AMP Robotics.

Real-Time Image Analysis to Rapid Screening

Tools

Develop framework for rapid assessment of feedstock fraction components to predict low-temperature conversion performance



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Description

- Predictive models to rapidly estimate biomass digestibility by constructing hybrid model architecture built with neural network models, which will quantify the degree of mechanical deconstruction, on top of physics-based models, which will account for intraparticle diffusion and hydrolysis kinetics.

Value of New Tools

- Allow biorefinery industries to quickly evaluate biomass quality, determine process parameters, and predict plant economics based on feedstock variabilities.
- Understand the effect of harvesting and air classification technology and strategy on downstream biomass composition and conversion.

Potential Customers & Outreach Plan

- Seeking collaboration opportunities to apply the model to real-time biomass used in SAFFiRE project with D3Max and Southwest Airlines.

MSW and CMAs for Conversion

Knowledge

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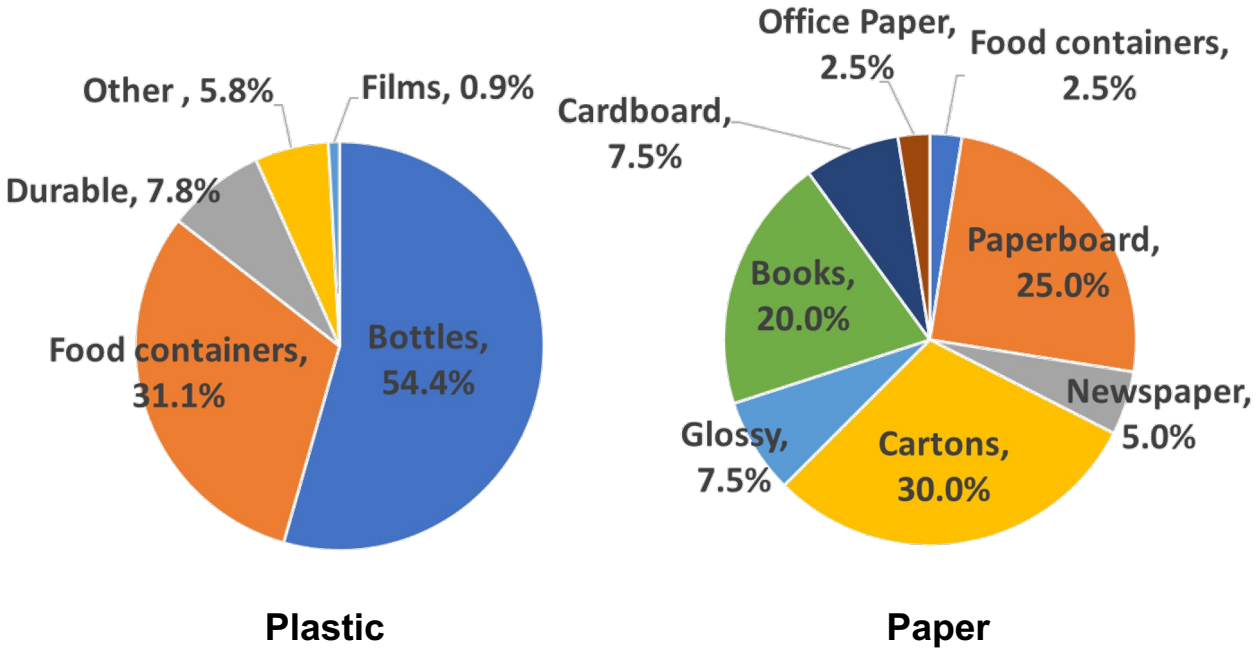
Provide a consistent source of MSW as an interface between FCIC work with MSW

Mass balance characterization



Plastic **Paper**

Description

- Residual MSW bales received from a single-stream recycling facility were deconstructed and hand-sorted by material type.

Achievement

- Created three MSW streams from the residual MRF materials: (1) as-received, (2) plastic-rich, and (3) paper-rich.
- Size reduced the streams to 4 mm or 2 mm and split to achieve desired amounts for shipping.
- Shipped requested MSW materials to other FCIC subtasks.

Relevance

- Provided CMA data on each MSW stream.
- Developed a processing method to provide a consistent source of MSW for other FCIC subtask experimentation.

Impact

Translate knowledge and tools into actionable resources for industry and collaborators.

- Methods developed in this task are already being directly leveraged via our project with Forest Concepts.

forestconcepts™ bioenergy

- Contributing to an undergraduate-level textbook on best practices in biomass comminution to educate the next generation of bioenergy engineers.
- Working with Resource Recycling Systems, an MSW consulting group, to obtain relevant waste materials from a single-stream material recovery facility in Ann Arbor, MI, and communicate preprocessing results.

RRS

- Exploring opportunities for collaboration with machine vision approaches such as WipWare and AMP Robotics.

WipWare AMP ROBOTICS™

Summary – Preprocessing

Technical Approach

Use multiscale experimental and modeling techniques to understand how material attributes and strength properties translate to comminution performance, and how critical attributes for conversion may be changed across preprocessing methods.

Impact

This subtask meets the objectives of the FCIC by developing transfer functions for deconstruction and process control that can be utilized by industry to develop new designs and operational maps for unit operations that meet CMAs for SAF.

Achievements

- **Understand and explore the origin of strength properties in biomass** with fundamental molecular/polymer- to particle-scale models and experiments.
- **Predict pilot-scale knife mill performance** across a range of sizes, moistures, and mill screens with empirically driven statistics and discrete particle models.
- Develop a framework to **rapidly assess biomass digestibility** with a framework for rapid analysis of fibers.
- Characterize and process **curated sample sets of MSW and biomass** for study across the consortium.

Quad Chart Overview

Timeline

- Project start date: October 1, 2021
- Project end date: September 30, 2024

	FY22 Costed	Total Award
DOE Funding	$2,075,000	$6,225,000

Project Goal

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

End of Project Milestone

Comminution manuals and robust process control models. The comminution manuals will contain design principles for various working envelopes of CMAs and CPPs for corn stover, forest resides, and MSW that reliably produce CQAs required for various downstream conversion processes. The process control model will utilize low-cost cameras to identify process upsets so downstream process parameters can be adjusted to avoid process upsets.

Funding Mechanism

2021 Lab Call – FCIC Merit Review

Impact

Publications:

1. Sun, Quan, Qiushi Chen, Yidong Xia, Feiyang Chen, Jordan Klinger, Ling Ding, and Vicki Thompson. "Reverse scaling of a bonded-sphere DEM model: Formulation and application to lignocellulosic biomass microstructures." *Powder Technology* 409 (2022): 117797.
2. Hamed, Ahmed, Yidong Xia, Nepu Saha, Jordan Klinger, David N. Lanning, and Jim Dooley. "Flowability of Crumbler rotary shear size-reduced granular biomass: An experiment-informed modeling study on the angle of repose." *Frontiers in Energy Research* (2022): 319.
3. Crowley, Meagan F., Hariswaran Sitaraman, Jordan Klinger, Francois Usseglio-Viretta, Nicholas E. Thornburg, Nicholas Brunhart-Lupo, M. Brennan Pecha, James H. Dooley, Yidong Xia, and Peter N. Ciesielski. "Measurement of Transport Properties of Woody Biomass Feedstock Particles Before and After Pyrolysis by Numerical Analysis of X-Ray Tomographic Reconstructions." *Frontiers in Energy Research* 10, no. NREL/JA-2800-81834 (2022).
4. Xia, Yidong, Jordan Klinger, Tiasha Bhattacharjee, and Vicki Thompson. "The elastoplastic flexural behaviour of corn stalks." *Biosystems Engineering* 216 (2022): 218-228.
5. Chen, Feiyang, Yidong Xia, Jordan L. Klinger, and Qiushi Chen. "A set of hysteretic nonlinear contact models for DEM: Theory, formulation, and application for lignocellulosic biomass." *Powder Technology* 399 (2022): 117100.
6. Sun, Quan, Yidong Xia, Jordan Klinger, Robert Seifert, Joshua Kane, Vicki Thompson, and Qiushi Chen. "X-ray computed tomography-based porosity analysis: Algorithms and application for porous woody biomass." *Powder Technology* 388 (2021): 496-504.
7. Xia, Yidong, Feiyang Chen, Jordan L. Klinger, Joshua J. Kane, Tiasha Bhattacharjee, Robert Seifert, Oyelayo O. Ajayi, and Qiushi Chen. "Assessment of a tomography-informed polyhedral discrete element modelling approach for complex-shaped granular woody biomass in stress consolidation." *Biosystems Engineering* 205 (2021): 187-211.
8. Guo, Yuan, Qiushi Chen, Yidong Xia, Jordan Klinger, and Vicki Thompson. "A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles." *Powder Technology* 385 (2021): 557-571.
9. Li, Yudong, Ling Tao, Nick Nagle, Melvin Tucker, Xiaowen Chen, and Erik M. Kuhn. "Effect of Feedstock Variability, Feedstock Blends, and Pretreatment Conditions on Sugar Yield and Production Costs." *Frontiers in Energy Research* (2022): 908.
10. Thornburg, Nicholas E., Ryan M. Ness, Meagan F. Crowley, Lintao Bu, M. Brennan Pecha, Francois LE Usseglio-Viretta, Vivek S. Bharadwaj et al. "Mass transport limitations and kinetic consequences of corn stover deacetylation." *Frontiers in Energy Research* 10 (2022): 144.
11. Li, Yudong, Xiaowen Chen, and David A. Sievers. "Modelling a compressible packed bed flow-through washing and deacetylation reactor for corn stover pretreatment." *Chemical Engineering Journal* 415 (2021): 128918.
12. Sarkar, Daipayan, Lintao Bu, Joseph E. Jakes, Jacob K. Zeiba, Isaiah D. Kaufman, Michael F. Crowley, Peter N. Ciesielski, and Josh V. Vermaas. "Diffusion in Intact Secondary Cell Wall Models of Plants at Different Equilibrium Moisture Molecular Plant Sciences Invited Departmental Seminar, Michigan State University, March 14, 2022.

Impact

The work in this task contributed to 12 peer-reviewed scientific publications and 10 presentations at society meetings and trade shows:

Presentations:

1. Klinger, Jordan, Tiasha Bhattacharjee, Yidong Xia, Ahmed Hamed, Peter Ciesielski, Yudong Li, Xiaowen Chen, Rebecca Brown, Neal Yancey, Vicki Thompson, and David Thompson. “Influence of Biomass Physical Properties and Comminution Techniques on Size Reduction Performance.” In *2023 International Biomass Conference and Expo*. Atlanta, GA, February 28, 2023.
2. Bhattacharjee, Tiasha, Jordan Klinger, Vicki Thompson, Yidong Xia, Susan Carilli, Monica Oliva-Sifuentes, Neal Yancey, and John E. Aston. "Scale-up of Corn Stover Comminution Population Balance in Knife Mills." In *2022 AIChE Annual Meeting*. AIChE, 2022.
3. Xia, Yidong, Jordan Klinger, Tiasha Bhattacharjee, John E. Aston, and Vicki Thompson. "The Elastoplastic Flexural Behavior of Corn Stalks: An Experiment-Informed DEM Model and Process Simulation of a Knife Mill." In *2022 AIChE Annual Meeting*. AIChE, 2022.
4. Klinger, Jordan, Neal Yancey, Rachel Emerson, Yidong Xia, Tiasha Bhattacharjee, Susan Carilli, and Vicki Thompson. "Air-Classification of Forest Residues for Beneficiated High Temperature Conversion Feedstock." In *2021 AIChE Annual Meeting*. AIChE, 2021.
5. Chen, Xiaowen, Nick Nagle, Ryan Davis, Ian McNamara, Eric Tan, and Ling Tao. "Lowering GHG emissions and minimum sugar selling price of DMR process with 2-stage Na2CO3 and NaOH Deacetylation." In *44th Symposium on Biomaterials, Fuels and Chemicals*. SIMB, 2022.
6. Bhattacharjee, Tiasha, Jordan Klinger, Susan Carilli, Vicki Thompson, and Neal Yancey. "Population Balance of Knife Milled Corn Stover." In *2021 AIChE Annual Meeting*. AIChE, 2021.
7. Ciesielski, P., Addison, B., Bharadwaj, V. , Crowley, M., and Crowley, M. “Multiscale modeling for conversion and catalytic upgrading of lignocellulosic biomass.” Invited plenary presentation, Frontiers in Biorefining, Simons Island, GA, October 24, 2022.
8. Ciesielski, P. “Elucidating Emergent Properties of Lignocellulosic Biopolymer Assemblies Through Macromolecular Modeling.” Invited oral presentation, Materials Research Society Fall Meeting, Boston, MA, November 28, 2022.
9. Ciesielski, P. “Multiscale Modeling for Bioenergy Applications.” Invited international presentation (virtual). ABISURE Network Meeting, Medellín, Colombia. June 22, 2022.
10. Ciesielski, P., Crowley, M., Bu, L., Bharadwaj, V., and Crowley, M. “Elucidating the Molecular Origins of Mechanical Properties of Biomass through Molecular and Coarse-Grained Dynamics Simulations of Lignocellulose Assemblies.” Molecular Plant Sciences Invited Departmental Seminar, Michigan State University, March 14, 2022.