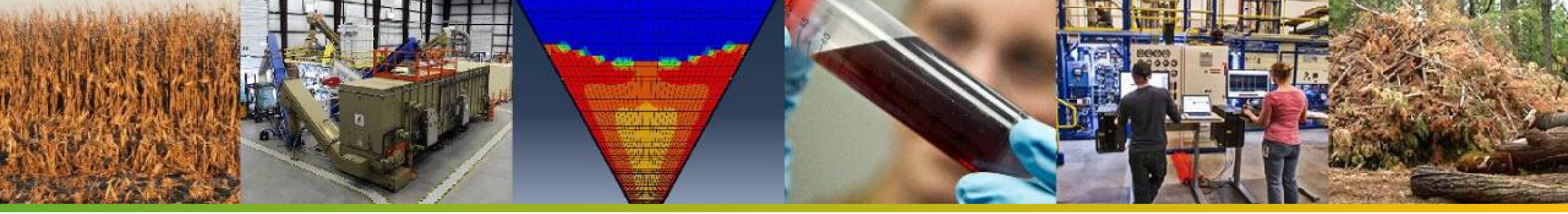


Lessons Learned in the Feedstock-Conversion Interface Consortium (FCIC)

April 14, 2021

Edward J. Wolfrum, Ph.D.
Principal Investigator

1-slide guide to the FCIC

fcic
FEEDSTOCK-CONVERSION
INTERFACE CONSORTIUM

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

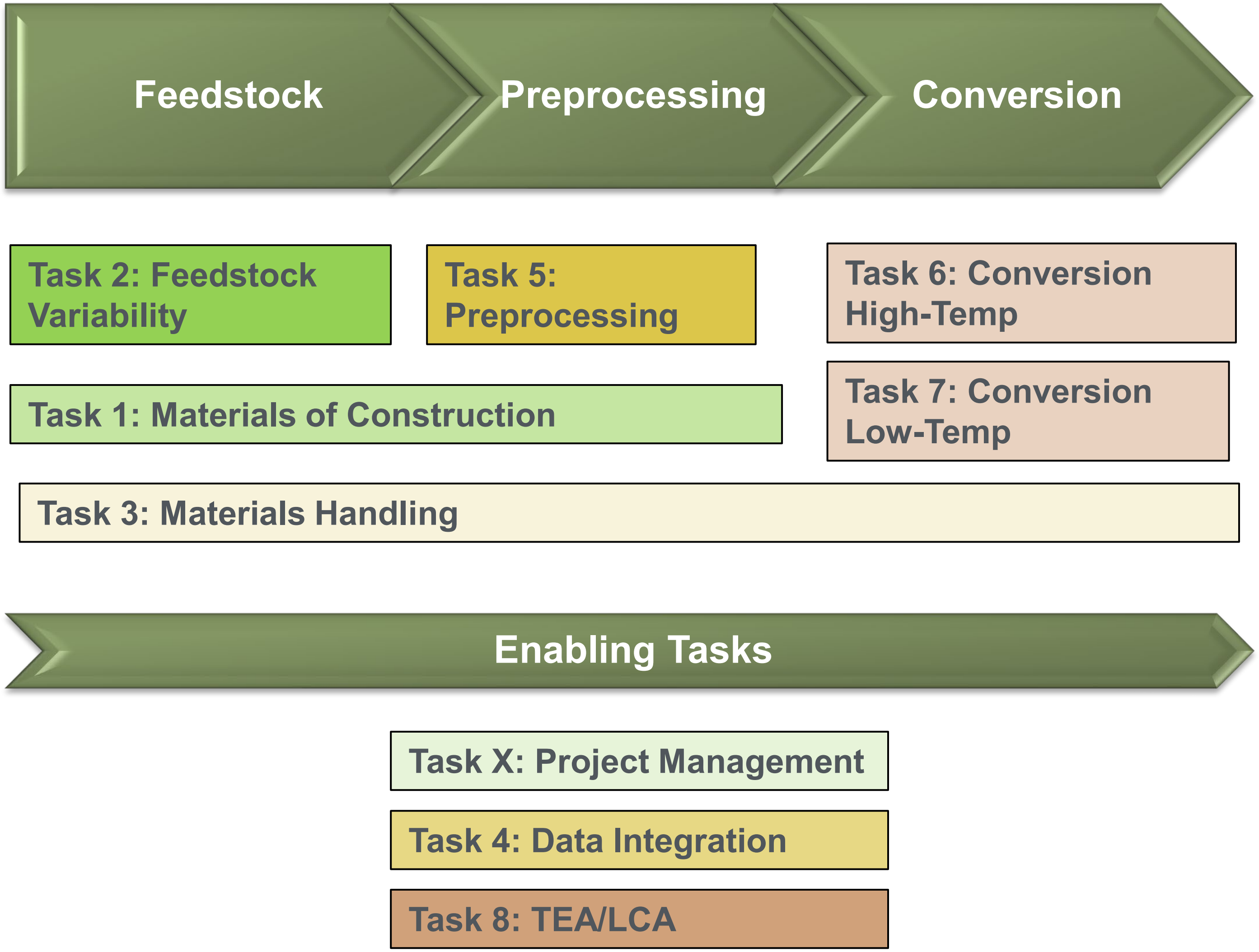
Key Ideas

- 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
BERKELEY LAB
OAK RIDGE National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
NATIONAL ENERGY TECHNOLOGY LABORATORY
NREL NATIONAL RENEWABLE ENERGY LABORATORY

FCIC Task Organization



Feedstock

Preprocessing

Conversion

Task 2: Feedstock Variability

Task 5: Preprocessing

Task 6: Conversion High-Temp

Task 7: Conversion Low-Temp

Task 1: Materials of Construction

Task 3: Materials Handling

Enabling Tasks

Task X: Project Management

Task 4: Data Integration

Task 8: TEA/LCA

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

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

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

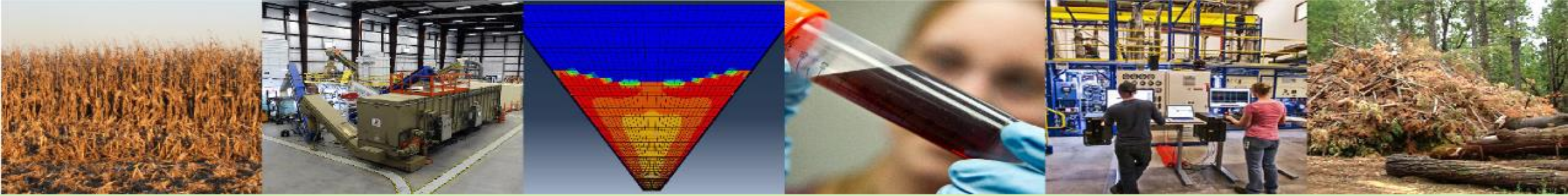
Task 3: Materials Handling: Develop tools that enable continuous, steady, trouble free feed into reactors

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

Task 6 & 7: Conversion (High- & Low-Temp Pathways): Produce homogeneous intermediates to convert into market-ready products

Task 8:Crosscutting Analyses TEA/LCA: Valuation of intermediate streams & quantify variability impact



Key Learnings

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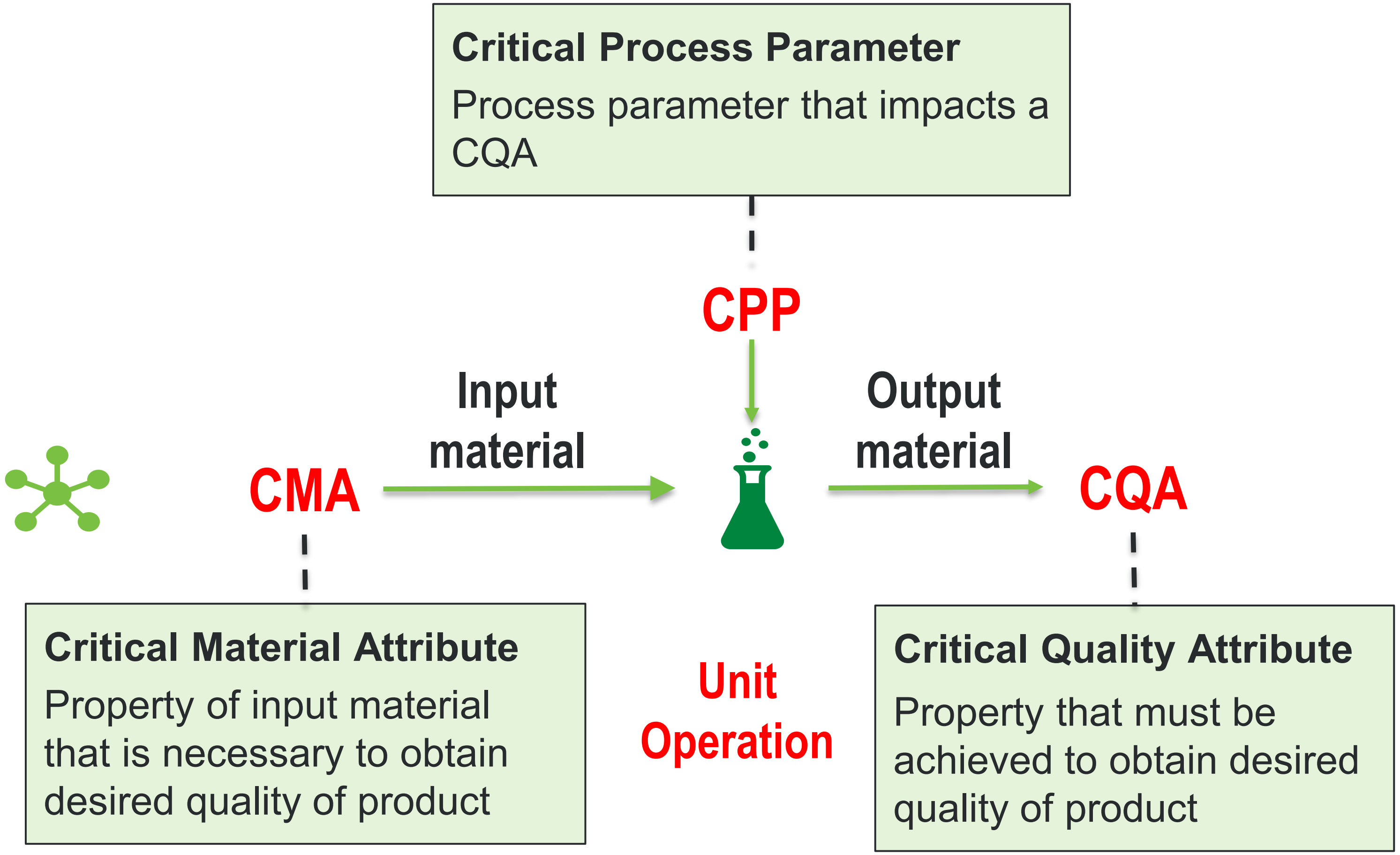
Quality by Design (QbD)

- 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
- Need fundamental understanding of
  - Unit operation
  - Input & Output streams


Critical Process Parameter

Process parameter that impacts a CQA

Critical Material Attribute

Property of input material that is necessary to obtain desired quality of product

Critical Quality Attribute

Property that must be achieved to obtain desired quality of product

QbD is about Feedstock Attributes….

- Moving from feedstock **NAMES** to feedstock **ATTRIBUTES**
- **Physical Attributes**
- **Chemical Attributes**
- **Mechanical Attributes**

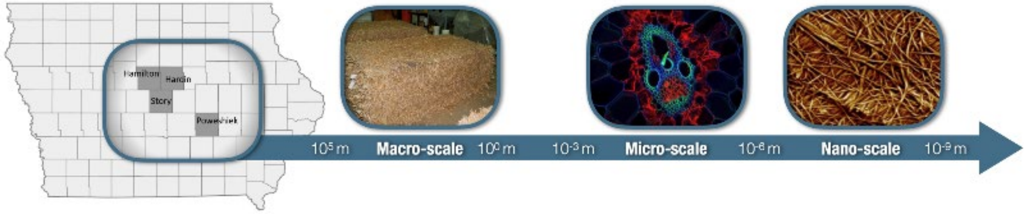


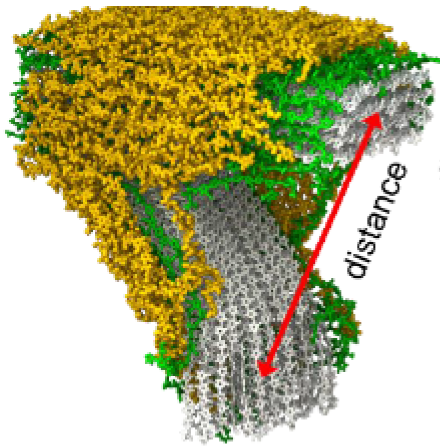


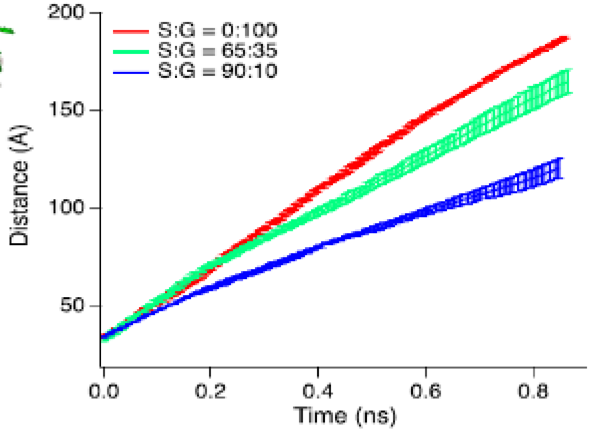
hayandforage.com

Critical Attributes Manifest at Different Scales

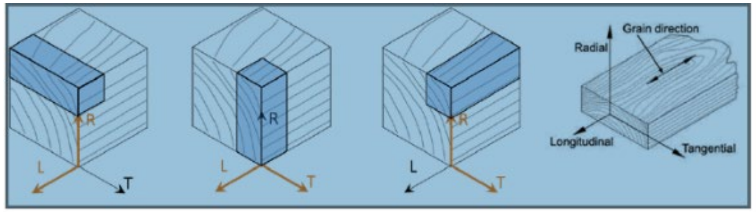
- Mechanical CMAs (stress/strain relationships) influence comminution performance
- Molecular-scale modeling suggests chemical composition can affect bulk scale mechanical CMAs

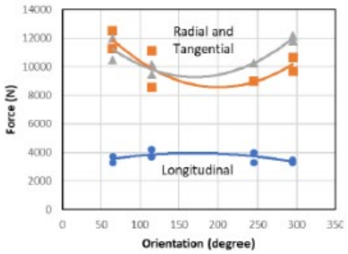


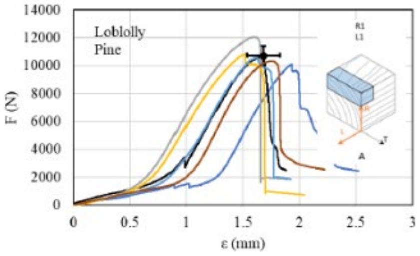




L-J potential	xylan/ s-lig	xylan/g-lig	xylan/h-lig	s-lig/s-lig	g-lig/g-lig	h-lig/h-lig
ε (kcal/mol)	24.27	20.91	15.35	24.10	22.00	17.31
r_m (Å)	4.13	4.53	3.95	4.76	3.43	4.49
r_0 (Å)	1.27	1.34	2.95	2.23	2.39	2.64

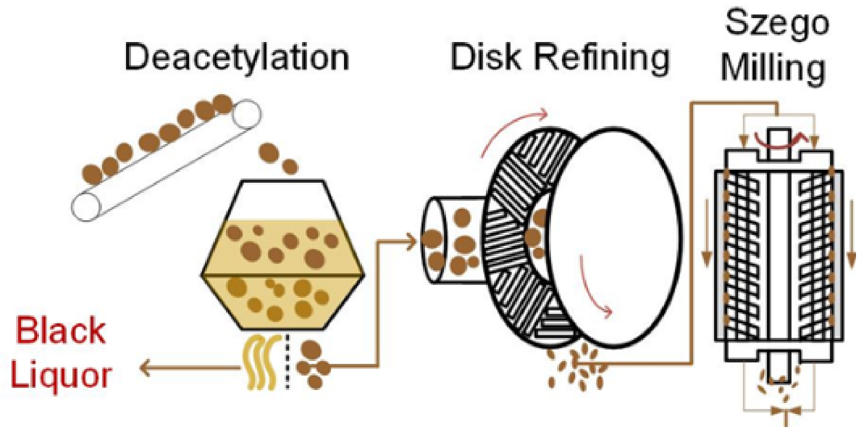


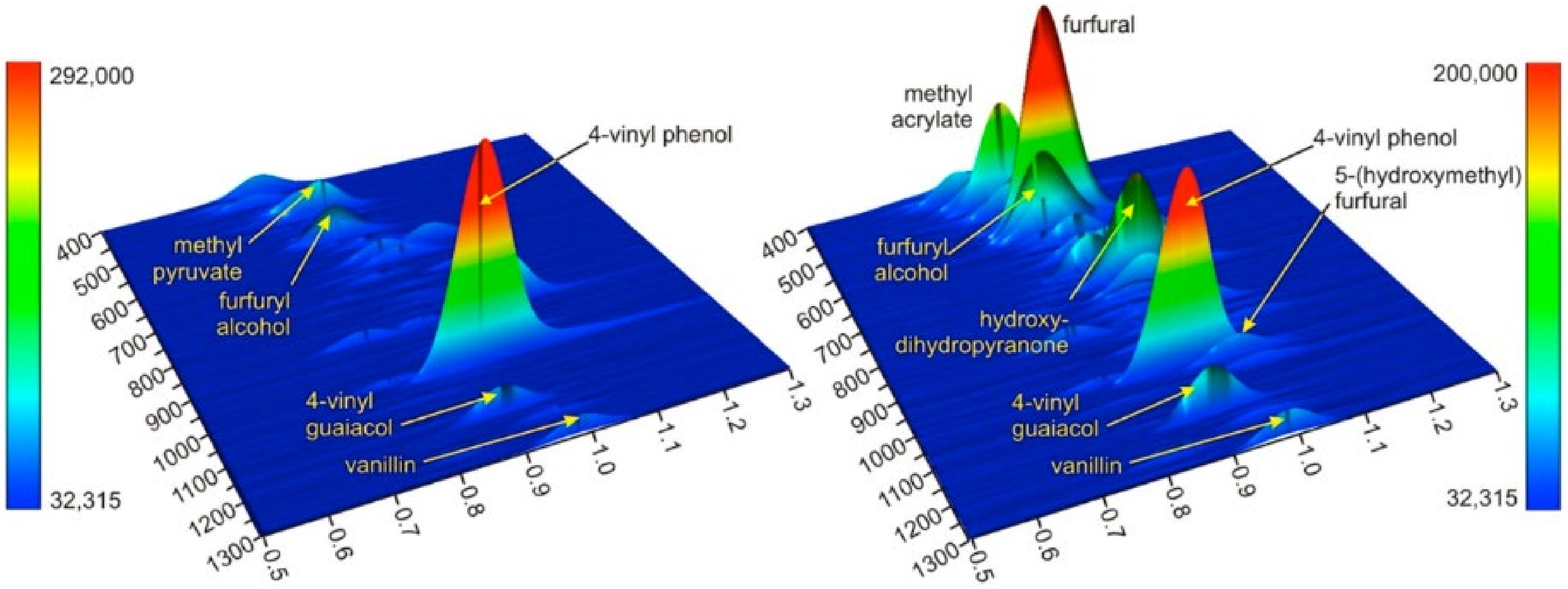




CQAs Can Skip Unit Operations

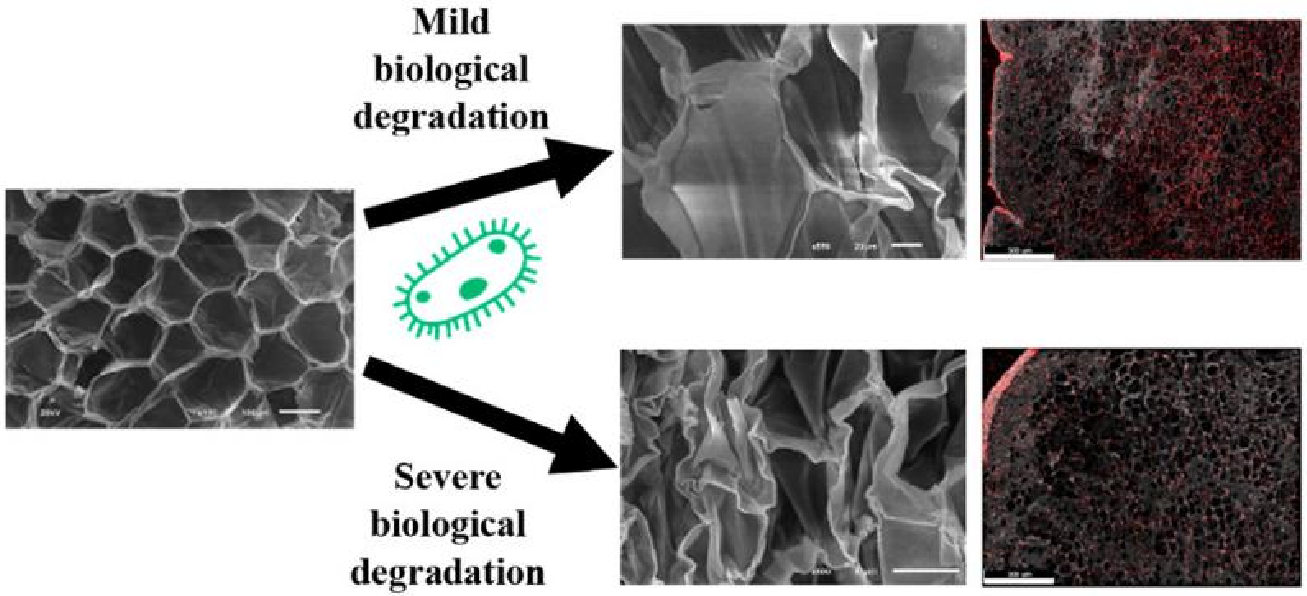
- Structural carbohydrates are influenced by genetics, harvest and storage
- They do not directly impact preprocessing but are critical in low-temperature conversion – ***yield is king***

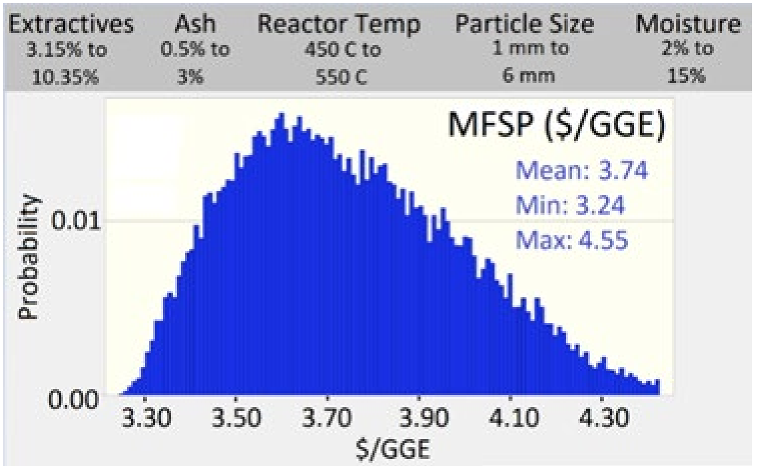




Critical Attributes Can Influence (and be Influenced by) Multiple Unit Operations

- Inorganics can be affected by harvest, storage, preprocessing unit operations
- Inorganics in woody materials affect fast pyrolysis yields
- Inorganics affect equipment wear in multiple unit operations

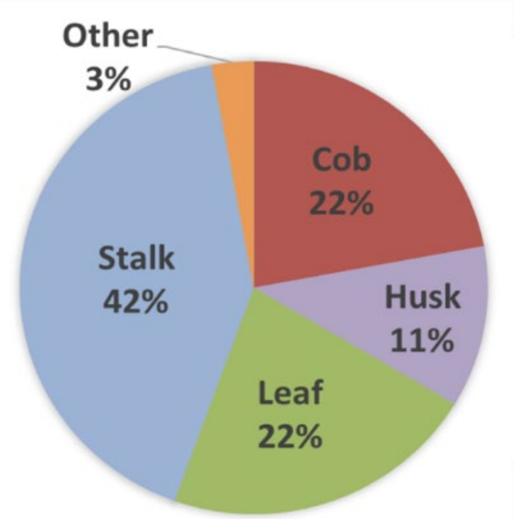




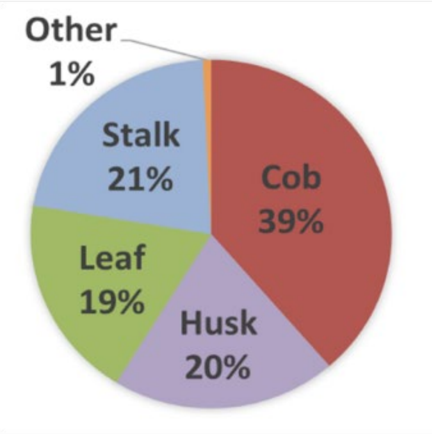
Investments in Preprocessing Can Yield Dividends in Conversion

- Corn Stover anatomical fractions show different yields in low-temperature conversion - DMR/EG
- Low-cost fractionation upstream will permit flexible conversion approaches – campaigning materials?

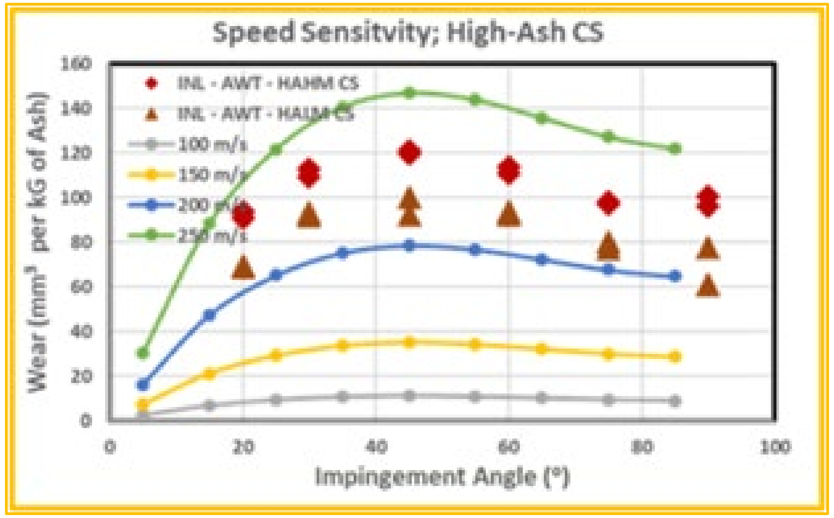
Whole Plant (above 6”)



Above Lowest Cob

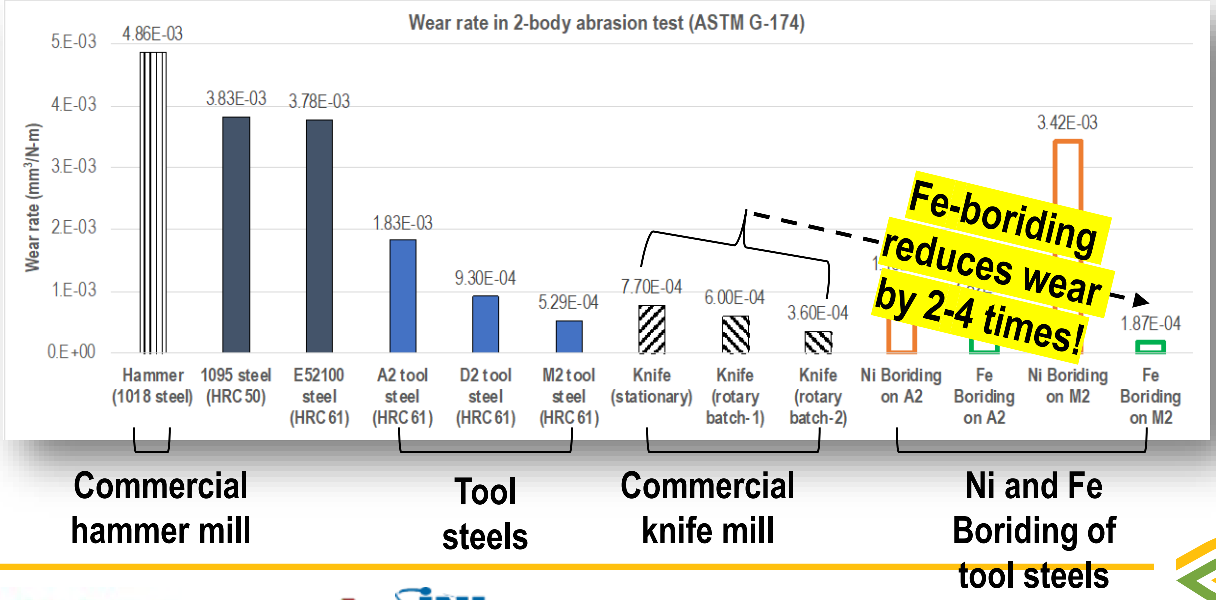


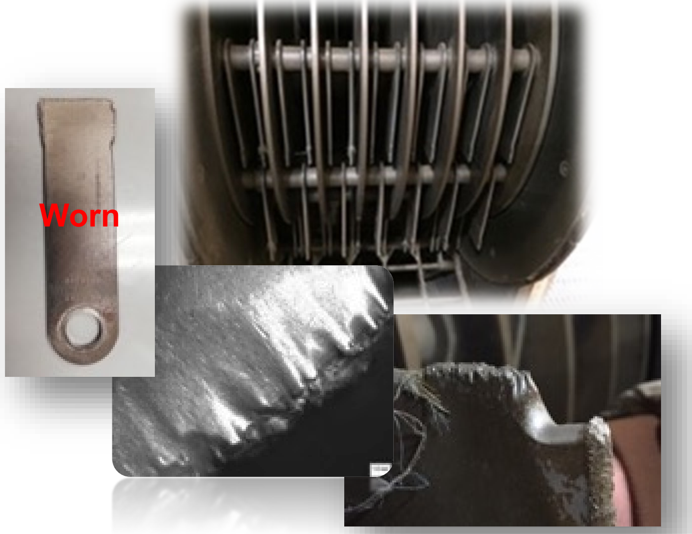
Material Wear in Processing Equipment can be Predicted and Mitigated



Mathematical models of erosive wear

- **validated against experimental data**
- **used to predict the** impact of feedstock CMAs, materials of construction, and process parameters (CPPs) on erosive wear





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

Ben-Ami erosion wear model

Questions?

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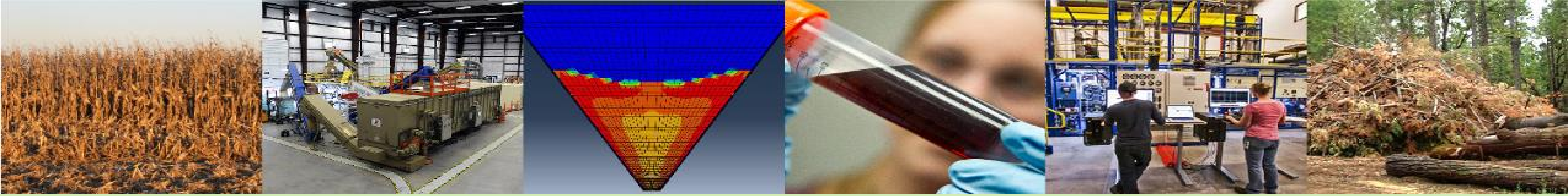

Additional Information on the FCIC

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

Throughput, Reliability, and Yields of a Pilot-Scale Conversion Process for Production of Fermentable Sugars from Lignocellulosic Biomass: A Study on Feedstock Ash and Moisture

David A. Sievers*, Erik M. Kuhn, Vicki S. Thomp

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Advances in Multiscale Modeling of Lignocellulosic Biomass

Peter N. Ciesielski*, M. Brennan Pecha, Aaron M. Lattanzi, Vivek S. Bharadwaj, Meagan F. Crowley, Lintao Bu, Josh V. Vermaas, K. Xerxes Steirer, and Michael F. Crowley

Cite this: ACS Sustainable Chem. Eng. 2020, 8, 9,

Publication Date: February 13, 2020

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Article Views 714 | Altmetric 8 | Citations 2

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*

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Article Views 277 | Altmetric - | Citations 6

SUBJECTS: Organic acids, Degradation, Aldehydes, Biomass, Pyrolysis

Material Characterization-Based Wear Mechanism Investigation for Biomass Hammer Mills

Sougata Roy, Kyungjun Lee, Jeffrey A. Lacey, Vicki S. Thompson, James R. Keiser, and Jun Qu*

Cite this: ACS Sustainable Chem. Eng. 2020, 8, 8, 3541−3546

Publication Date: February 20, 2020

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Article Views 203 | Altmetric - | Citations -

Pilot Plant Reliability Metrics for Grinding and Fast Pyrolysis of Woody Residues

Jordan Klinger, Daniel L. Carpenter*, Vicki S. Thompson, Neal Yancey, Rachel M. Emerson, Katherine R. Gaston, Kristin Smith, Michael Thorson, Huamin Wang, Daniel M. Santosa, and Igor Kutnyakov

Cite this: ACS Sustainable Chem. Eng. 2020, 8, 7, 2793−2805

Publication Date: January 20, 2020

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Article Views 289 | Altmetric - | Citations 1

A Review of Computational Models for the Flow of Milled Biomass Part II: Continuum-Mechanics Models

Wencheng Jin*, Jonathan J. Stickel*, Yidong Xia, and Jordan Klinger

Cite this: ACS Sustainable Chem. Eng. 2020, 8, 16, 6157−6172

Publication Date: April 3, 2020

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Article Views 209 | Altmetric - | Citations 2

SUBJECTS: Biomass, Stress, Granular materials, Fluid dynamics, Materials

Abstract

The design of efficient material handling systems for milled lignocellulosic biomass is challenging due to their complex particle morphologies and frictional interactions. Computational modeling, including the discrete element method (DEM) and continuum-based finite element/volume methods, may offer scientific insight and predictive capabilities for the flow of milled biomass in hoppers and feeders. This article (Part II) presents a review of current state-of-the-art continuum models for the flow of milled biomass, whereas DEM models are reviewed in a companion article (Part I). Advances of numerical methods to solve the global governing equations are discussed first, followed by a comprehensive review of constitutive models for granular materials, including Drucker–Prager, hypoplastic, Cambridge-type, inertial-rheology, and nonlocal granular fluidity models. Specifically, we provide in depth discussion on the suitability of those models for milled lignocellulosic biomass materials in terms of nonlinear elasticity, dependence of flow strength on pressure, density and shear rate, and compaction (dilation) associated with hardening (softening). Our study shows that, despite the recent advances in continuum granular flow modeling, the most suitable constitutive models still need further development to account for material parametrization, multiflow regimes, and multiscale behavior before they can be reliably used to optimize the design and operation of biomass handling systems.

Applied Energy

Volume 241, 1 May 2019, Pages 25-33

High-Octane Gasoline from Biomass: Experimental, Economic, and Environ Assessment

Daniel P. Dupuis, R. Gary Grim, Eric Nelson, Eric C.D. Tan, Daniel A. Rud, Tyler Westover, Jesse E. Hensley, Daniel Carpenter

https://doi.org/10.1016/j.apenergy.2019.02.064

Highlights

- Syngas compositions, heating values, and yields were ind feedstock.
- Syngas from blended feedstocks follows a linear mix of th feeds.
- Miscanthus is the most cost-effective feedstock to produc fuels.
- Forest residues has the lowest associated life-cycle carbon

Powder Technology

Volume 368, 15 May 2020, Pages 45-58

A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine

Wencheng Jin, Jordan L. Klinger, Tyler L. Westover, Hai Huang

https://doi.org/10.1016/j.powtec.2020.04.038

Highlights

- Drucker-Prager/Cap model is used for modeling shear behavior of ground loblolly pine.
- Oedometer and shear experiments were conducted and used to calibrate the parameters.
- Simulations identify the triaxial compression stress state inside the shear plane.
- Simulation results of Mohr-Coulomb envelopes agree well with experimental data.

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

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Feedstock Variability Task

Objective:

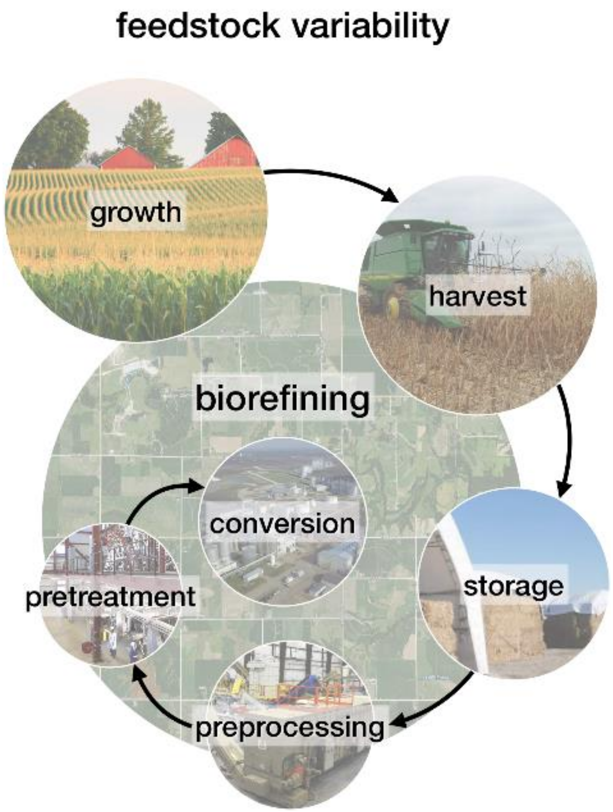
- Identify & quantify the initial distribution of feedstock CMAs and inform strategies to reduce and manage this variability

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.



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.

of arbitrary shapes

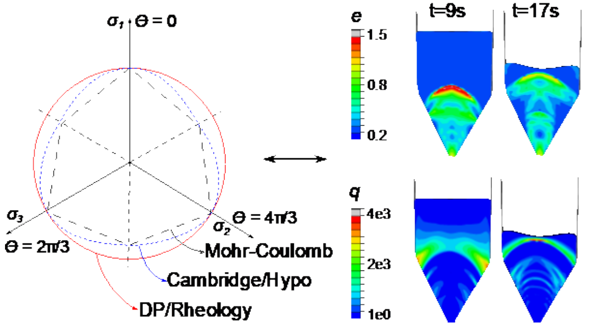
A v-shape hopper discharge simulation

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

Preprocessing Task

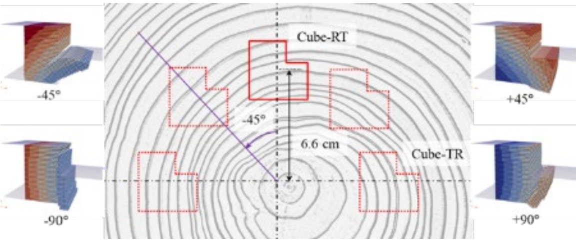
Objective: Develop science-based design and operation principles informed by TEA/LCA that result in predictable, reliable and scalable performance of preprocessing unit operations.

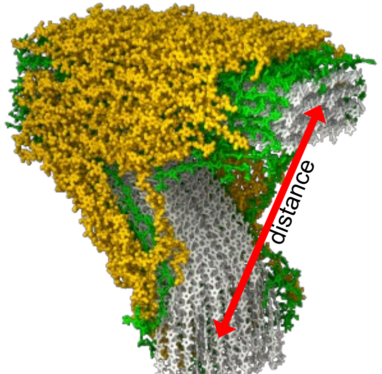
Impact: This task will provide knowledge and tools to pioneer biorefineries and other industry stakeholders through fundamental studies of comminution, fractionation, and deacetylation that produce validated mechanistic models.

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.





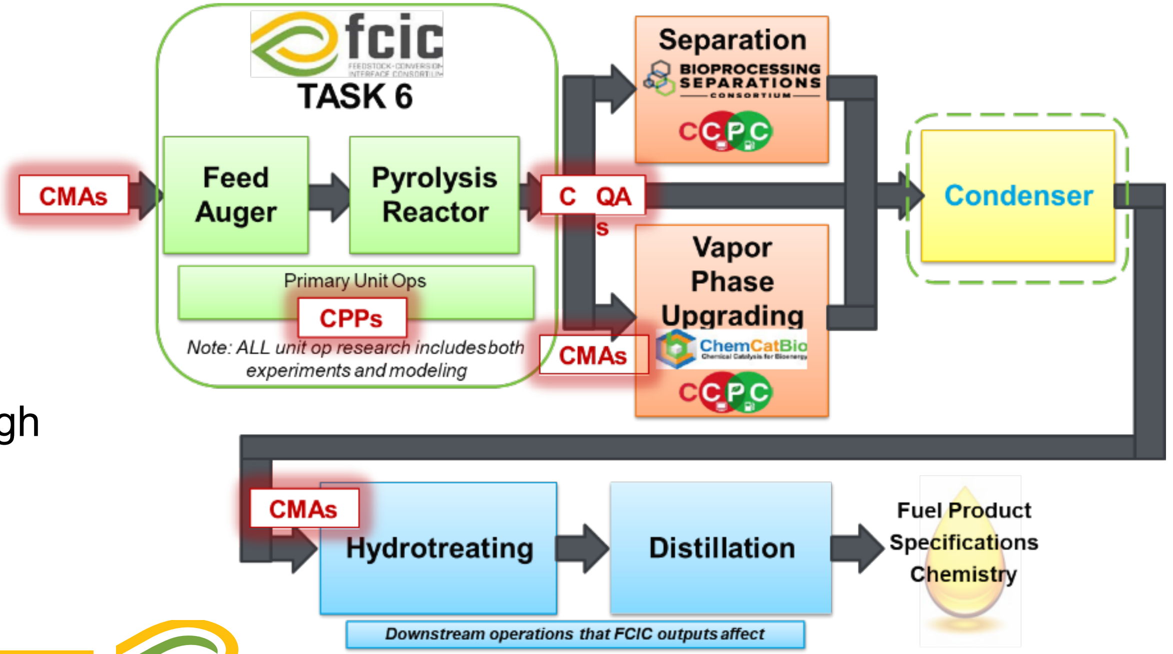
High Temperature Conversion Task

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.

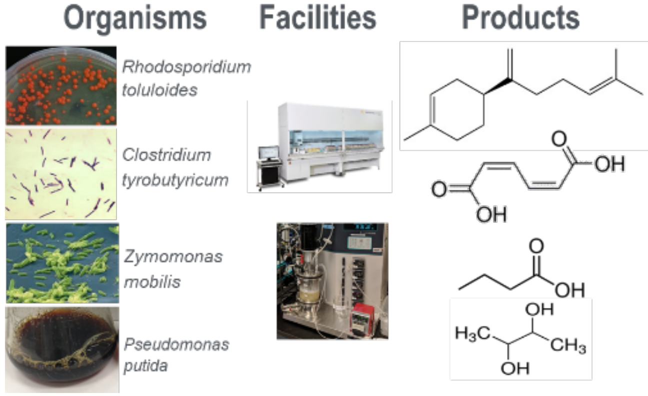


Low Temperature Conversion Task

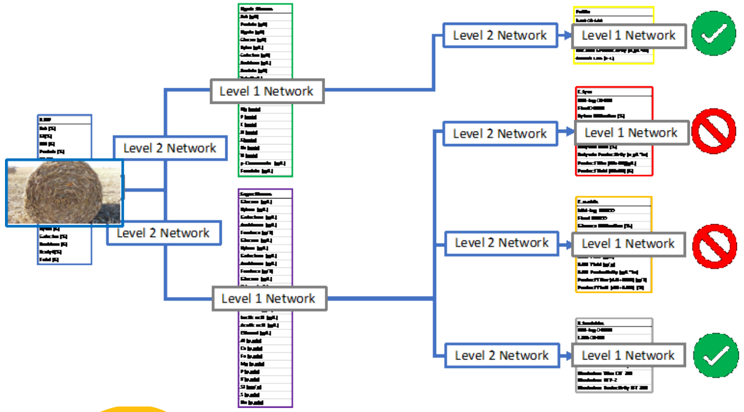
Objective: Determine the effects of biomass feedstock variability on the low-temperature conversion process chain (both sugar and lignin pathways) and develop tools to mitigate the risks posed by this variability.

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.



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

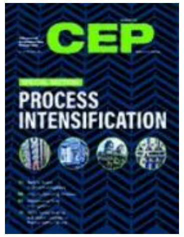
Potential Customers & Outreach Plan:

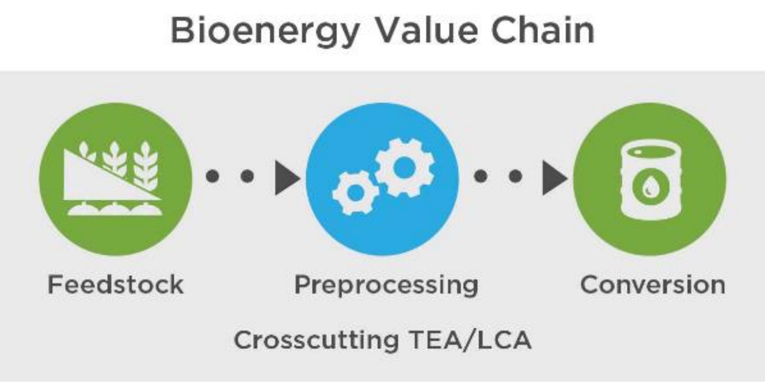
- Customers are bioenergy industry stakeholders across the value chain
- Engaging FCIC IAB for feedback on case study formulation, approach, assumptions
- 1-pagers highlighting highest impact case studies on FCIC website
- Conference presentations and associated trade journals

INTERNATIONAL POWDER & BULK SOLIDS CONFERENCE & EXHIBITION

ASABE

AIChE

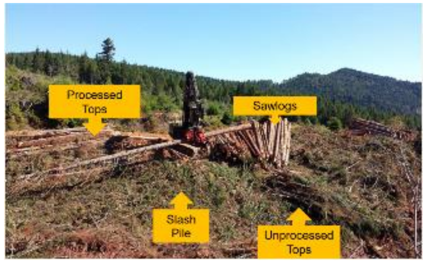


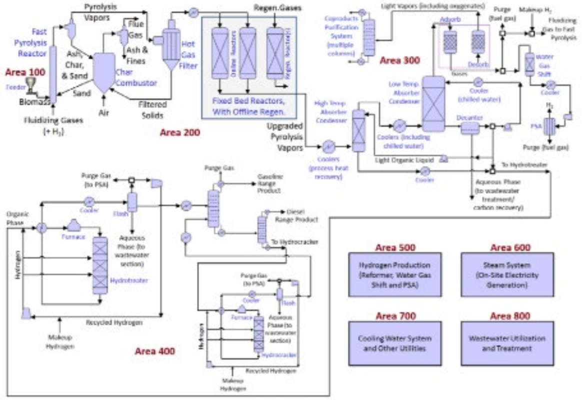


Bioenergy Value Chain

Feedstock → Preprocessing → Conversion

Crosscutting TEA/LCA



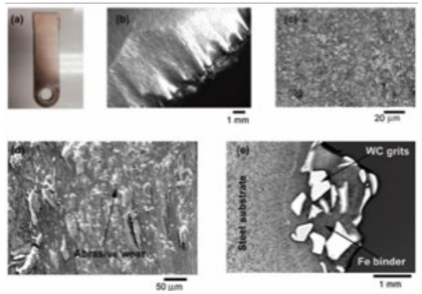


Materials of Construction Task

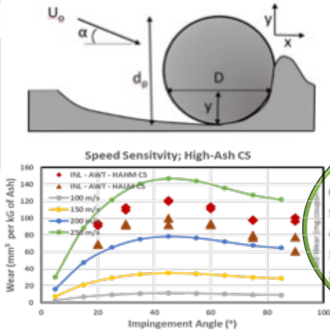
Objective: Using integrated efforts of characterization, modeling, and testing to gain fundamental understanding of failure modes and wear mechanisms, develop analytical tools/models to predict wear and establish material property specifications, select and evaluate candidate mitigations, and share the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

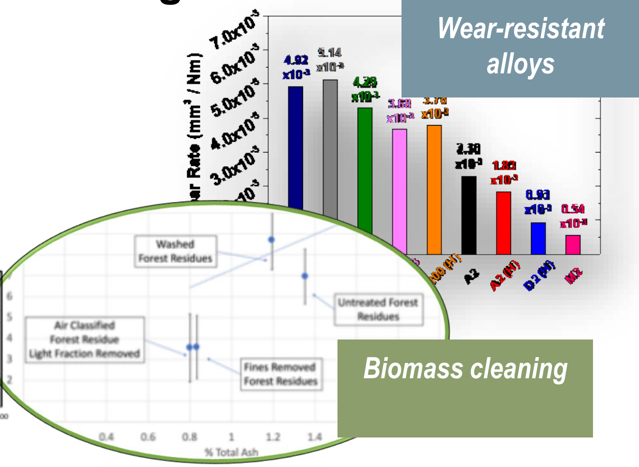
Characterize Wear



Model Wear



Mitigate Wear



Wear-resistant alloys

Biomass cleaning

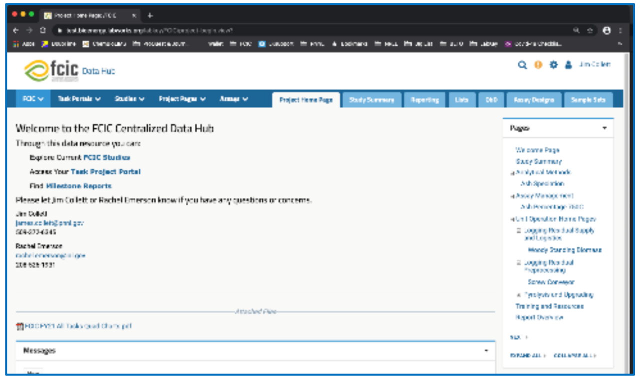
Outcome: Develop knowledge and tools to understand how to measure, predict, and mitigate wear.

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.

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.



Welcome to the FCIC Centralized Data Hub

Through this data resource you can:

Explore Current **FCIC Studies**

Access Your **Task Project Portal**

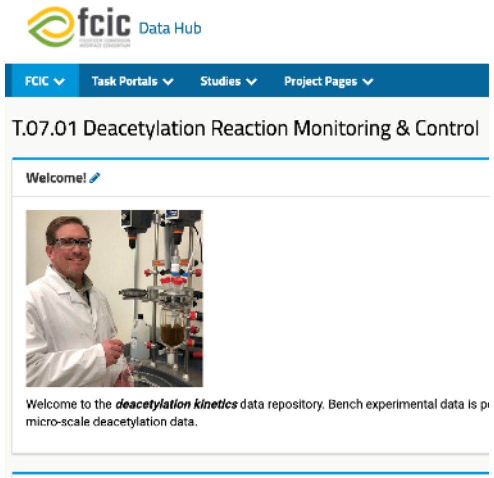
Find **Milestone Reports**

Please let Jim Collett or Rachel Emerson know if you have any questions or concerns.

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.



T.07.01 Deacetylation Reaction Monitoring & Control

Welcome!

Welcome to the ***deacetylation kinetics*** data repository. Bench experimental data is p
micro-scale deacetylation data.