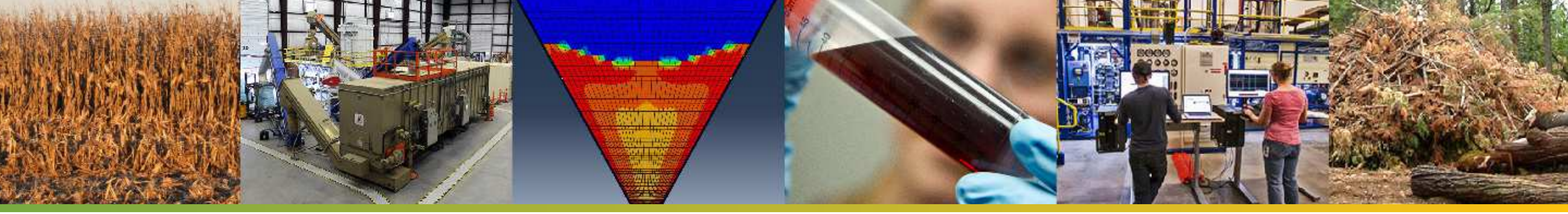


DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

FCIC Task 3 – Material Handling

Date: March 15, 2021
Feedstock-Conversion Interface Consortium

Yidong Xia (Task Lead), INL
Troy Semelsberger (Task Co-Lead), LANL

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

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

Task Team

Idaho National Laboratory

Luke Williams, Ph.D.; Wencheng Jin, Ph.D.; Yidong Xia, Ph.D.; Jordan Klinger, Ph.D.; Tiasha Bhattacharjee; Aaron Wilson, Ph.D.; Feiyang Chen (Clemson U)

National Renewable National Laboratory

Jonathan Stickel, Ph.D.; Syed Ahsan, Ph.D.; Hariswaran Sitaraman, Ph.D.; Mohammad Rahimi, Ph.D.; Jim Lischeske; Jessie Troxler (CSM)

Los Alamos National Laboratory

Troy Semelsberger, Ph.D.; Juan Leal, Ph.D.; (Lily) Ziwei Cheng, Ph.D.; Travis Rouse (Post Bac); Estrella Torres (UGS)

Argonne National Laboratory

Oyelayo Ajayi, Ph.D.; George Fenske, Ph.D.

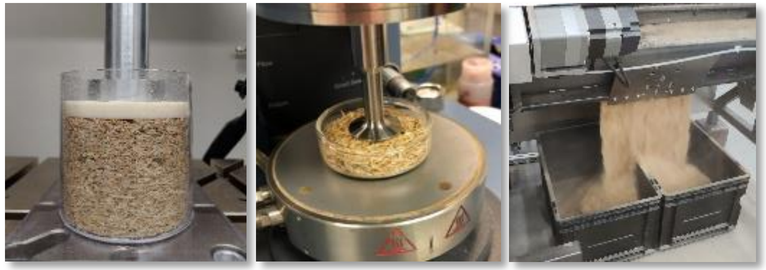
Pacific Northwest National Laboratory

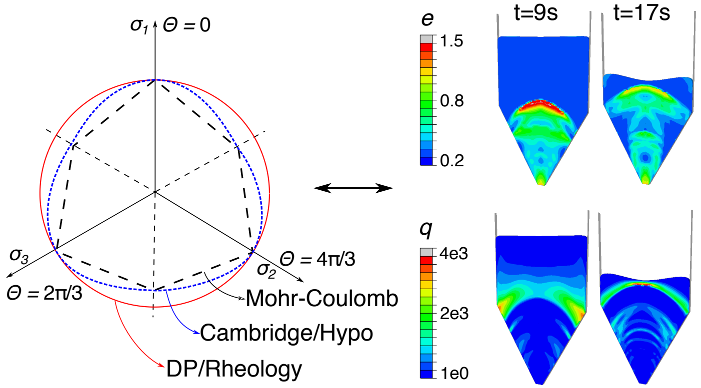
Richard Daniel, Ph.D.

Project Overview

- **Objective:** The objective of Task-3 Material Handling is to develop first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat.
- **Current limitations:** Current industry design practices perform empirical flow tests to modify existing equipment. Bulk solids handling consultants perform simple property characterization techniques (i.e., powders and soils), using empirical correlations to arrive at proposed geometries, which have, at best, limited utility with raw biomass.
- **Relevance:** This task supports the FCIC objective by developing physics-based modeling tools and supporting feedstock measurements and flow experiments for reliable feeding and handling solutions. This task will provide biomass industry with suitable & predictive design tools to assist design of feedstock processing & handling equipment.
- **Risks:** 1) Timely adaptation of handling equipment design to meet market interest & priority and maximize impact; 2) synergistic R&D and management across multiple R&D disciplines and Tasks in FCIC.

particles | of arbitrary shapes | discharge simulation





Project Overview (continued)

Relevance to TEA/LCA:

- Commercial-scale conversion of biomass in biorefineries has remained limited.
- A primary challenge in the design of a biorefinery is the storage, transport, and reactor feeding of the biomass feedstocks.
- Milling and handling have been prone to process upsets such as jamming and clogging, resulting in increased downtime and ultimately higher costs.

1 – Management

FY19-FY20: 3.1-3.6

FY21: 3.1, 3.3, 3.5, 3.7 (after reorganization).

Subtask	Lead(s)	Major Responsibilities
3.1: Continuum Modeling for Feedstock-Handling Equipment Design and Optimization	L. Williams (INL); J. Stickel (NREL)	Continuum models & computational tools for hopper feeding systems.
3.2: CFD Modeling for Reliable Operation of Screw Feeders **[Reorganized to 3.1 & 3.3 in FY21]**	J. Stickel (NREL)	Computational fluid dynamics (CFD) models and tools for compressible screw feeders.
3.3: Discrete Element Models for Fundamental Particle Flow Physics & Upscaling	Y. Xia (INL)	Particle models & computational tools for biomass particle physics.
3.4: Particle Friction and Cohesion Measurement **[Reorganized to 3.7 & 3.3 in FY21]**	O. Ajayi (ANL)	Particle-particle friction and particle-wall friction.
3.5: Bulk Material Characterization	J. Klinger (INL)	Physical and mechanical properties of biomass flow behavior in hoppers and augers. Determine critical material attributes and process parameters for hopper feeding systems.
3.6 Porosity & Pore Volume (CMA/CQA) **[Reorganized to 3.7]**	T. Semelsberger	Micro-porosity, meso-porosity, pore size distribution, pore volume of feedstocks.
3.7: Particle-Scale Property Measurements **[New in FY21]**	T. Semelsberger (LANL); O. Ajayi (ANL)	Quantify and correlate particle-scale property measurements of anatomical fractions.

1 – Management (continued)

- **Risks:** Lack of synergy between experimentalists and modelers, between the tasks, and between laboratories and industry.

  Task-3 has been mitigating the risks by 1) involving modelers in experimental design and testing, and 2) engaging in routine communication with the community and stakeholders.

- **Communication strategy:**
  - FCIC PIs, Task Leads, LRMs, and BETO TMs monthly meetings
  - Three Task-3 meetings per month
    - Task-3 monthly all-hands meetings
    - Task-3 monthly modeling progress meetings
    - Task-3 monthly experiment progress meetings
  - Participation in peer Tasks' meetings
    - Task-2 Feedstock Variability monthly meetings
    - Task-5 Preprocessing bi-weekly meetings
    - Task-6 & 7 (Conversion) progress meetings
  - Laboratory-industry partnership meetings (e.g., DFO project meetings and industry outreach)
  - FCIC topical webinar presentations (e.g., FCIC Modeling, Feb 2021) and Q&As

2 – Approach

Technical Approach: An integrated multiscale experimental and physics-based modeling approach (**also see a diagram in the next slide**):

- Controlled particle and bulk flow tests using industry-relevant biomass feedstocks and for evaluating flow performance under various combinations of CMAs and CPPs.
- Experiment-validated, physics-based discrete element models (DEM) for fundamental understanding of flow characteristics and upscaling of first-principles-based constitutive models as input to continuum flow models.
- Experiment-validated, physics-based continuum finite element and finite volume models (FEM & FVM) for predictive studies of engineering-scale flow performance under relevant combinations of CMAs and CPPs.
- Experimental and simulation data will be organized into LabKey to manage data flow among all subtasks and correlate biomass flow performance with CMAs and CPPs.

Challenges: 1) How to adapt experimental design to meet market interest & priority and maximize impact; 2) how to de-risk uncertainties in the predictability & robustness of the developed computational models.

FCIC Material Handling Task is a partner in BETO Consortium for Computational Physics and Chemistry (CCPC)

CCPC Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

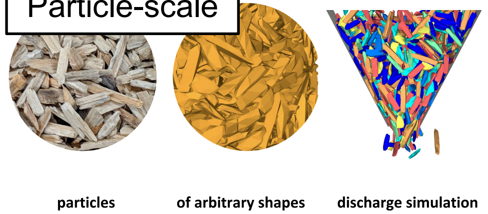
2 – Approach (continued)

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

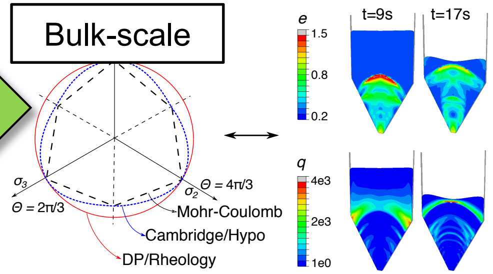
Experimental: multi-scale material characterization for state-of-the-art **knowledge** and **design charts**

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

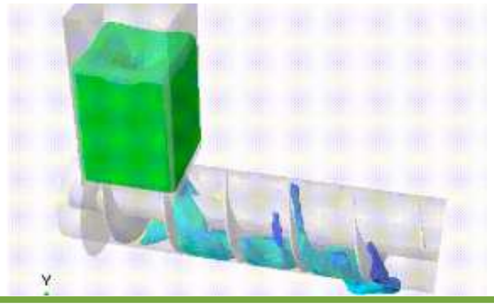
Particle-scale



Bulk-scale



Pilot/demonstration-scale



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

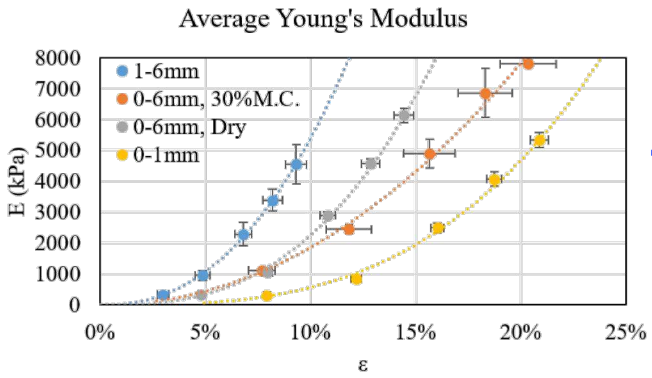
2 – Approach (continued)

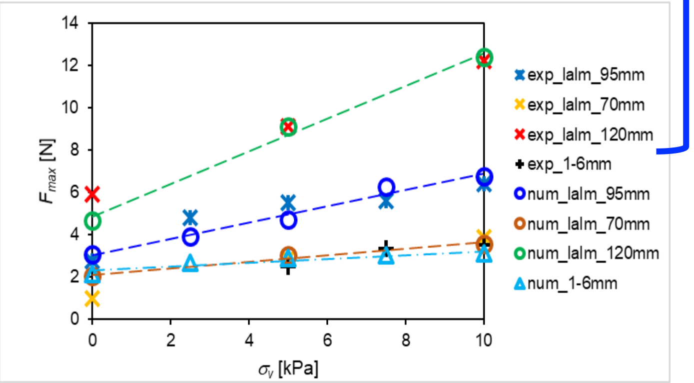
Metrics: 1) Operational reliability (e.g., design chart for consistent hopper flow at designed flow rate). 2) qualification of flow models (80% or higher agreement with experimental data (Go/No-Go milestone).

Example: hopper design – experiment-validated modeling investigation of MA, PP influence on CQA

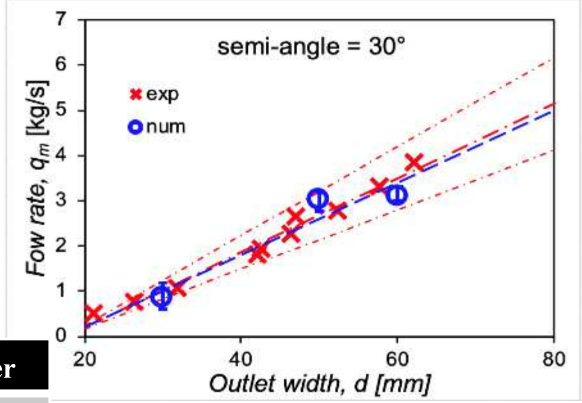
MA
Controllable attributes
Particle size distribution
Morphology (aspect ratio, shape, etc.)
Particle density/porosity
Surface energy
* Moisture content; * Ash content
Physical properties
Initial & critical state void ratio/density (bulk scale)
Critical state friction angle (bulk scale)
Elasticity (bulk scale)
Contact laws (particle scale)
* Time consolidation; * Scale-up effect

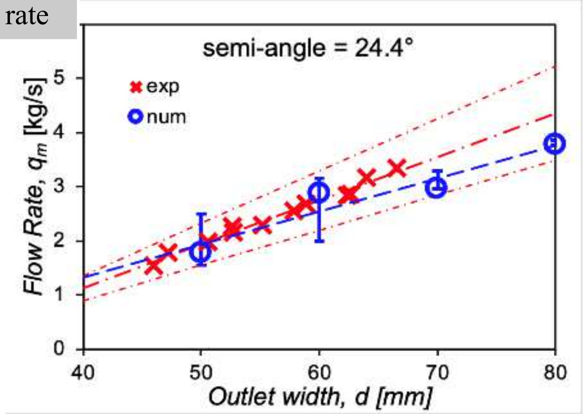
CPPs of Hopper
Feeding mass rate
Outlet mass rate
Depth
Side inclination angle
Outlet aperture size





CQAs of Hopper
Consistent flow at designed mass rate





Attributes denoted by * means not being currently studied in modeling

3 – Impact

Impact: This task will provide biomass industry with suitable & predictive design tools to effectively assist design of feedstock processing & handling equipment, including

- Reliable working envelope of critical material attributes (CMAs) & critical processing parameters (CPPs) for achieving critical quality attributes (CQAs) (i.e., design charts for consistent flow),
- Open-source biomass flow modeling software packages/moduli available to public.

Dissemination (list of publications and presentations in the additional slides)

Journal publications — **Conference proceedings** — **Industrial partnerships** — **Open-source software** — **Academia**

State of the art

ASABE

2020 AIChE ANNUAL MEETING

POWDER BULK SOLIDS THE POWDER SHOW DIGITAL FLOW

Demonstration

Outreach

forestconcepts™ bioenergy

JENIKE & JOHANSON SCIENCE ENGINEERING DESIGN

Demonstration

Collaboration

Available on GitHub

Education

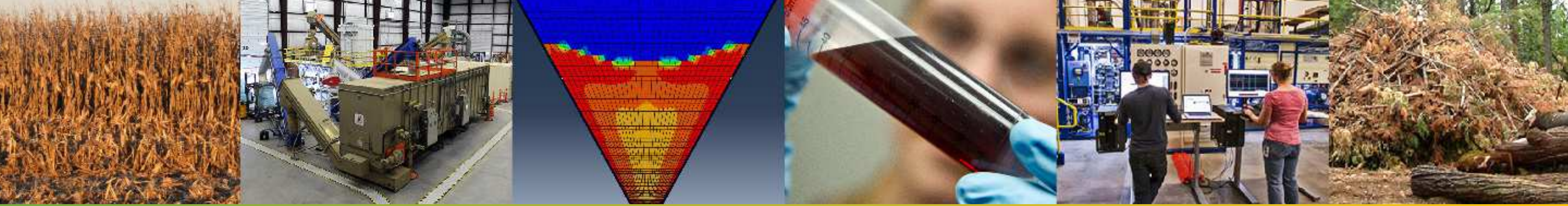
Contribution

Georgia Tech

COLORADO SCHOOL OF MINES EARTH • ENERGY • ENVIRONMENT

CLEMSON UNIVERSITY

Pathway to technology commercialization



4 – Progress and Outcomes

Outline

- **Modeling accomplishments**
  - Particle models
    - Complex-shape particle model
    - Coarse-grain particle model
    - Particle-air flow coupling model
  - Bulk flow models
    - Hopper and conveyer flow model
    - Compressible-screw feeder model
    - 1D pyrolysis screw-auger model
- **Experimental accomplishments**
  - Multiscale bulk flow characterization
    - Pilot scale
    - Laboratory scale
    - Microscale
  - Friction measurement
  - Porosity, pore volume & density measurement

Flow Models: Limitations & Best Practices

Knowledge

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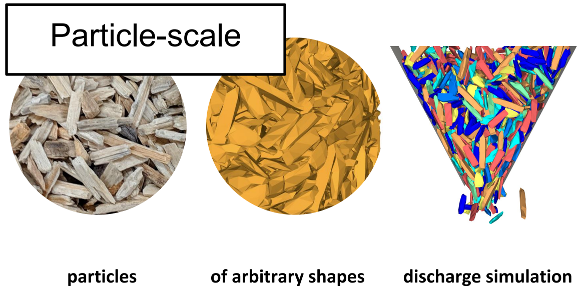
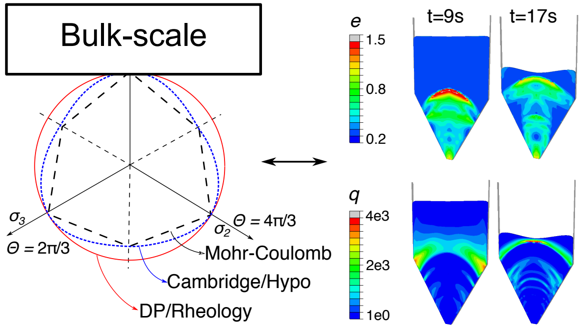
Identified particle- & bulk-scale models suitable for the flow of milled biomass and recommended best practices



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



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 new model development
- Lack of open-source model platforms for user coverage

Achievement

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

Relevance

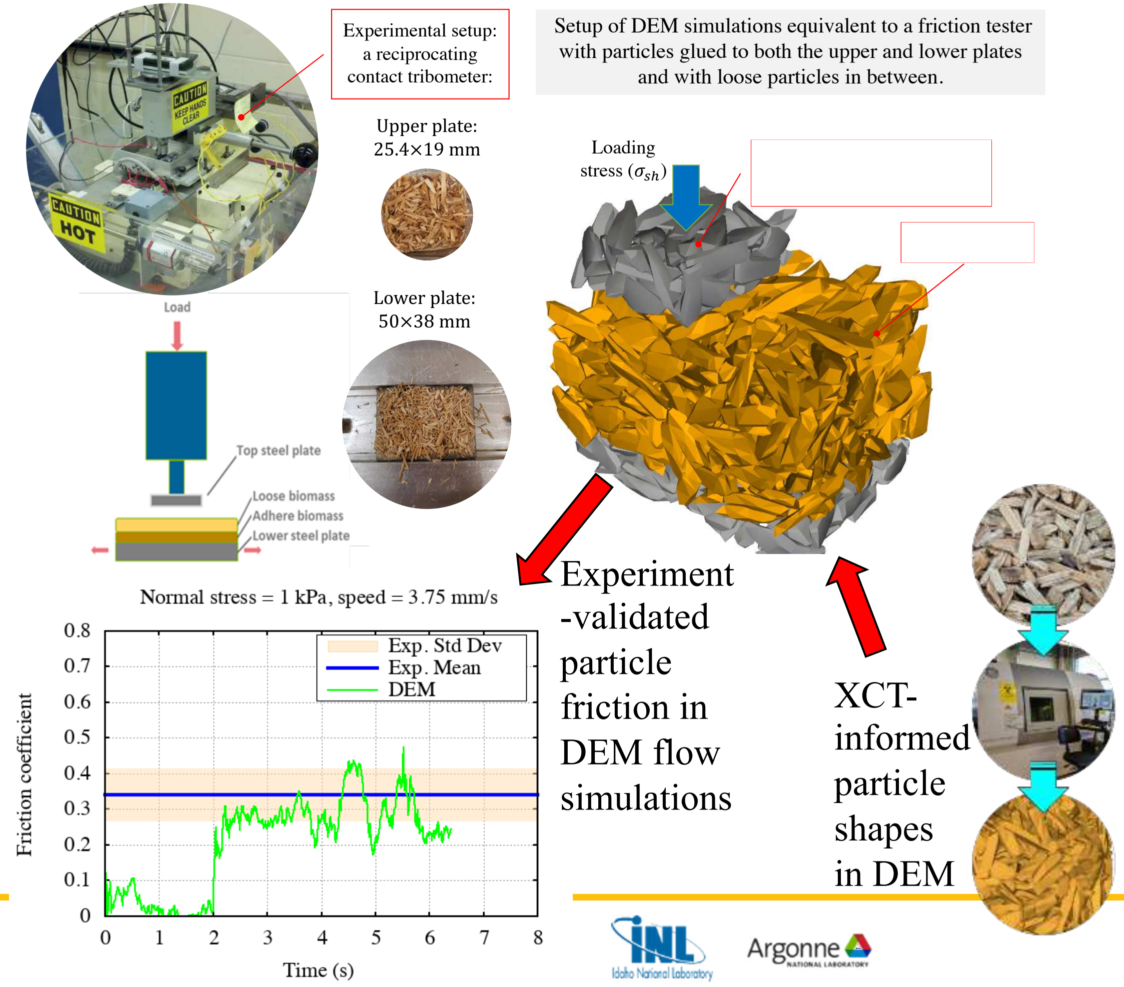
- Stakeholders in the bioenergy industry and academia will avoid wasting investment in modeling techniques not suitable for biomass
- Multiple invited presentations at ASABE AIM (Summer 2020)
- Invited to lead panel discussion at the International Powder & Bulk Solids Conference and Exhibition (Fall 2020)

Print version

Polyhedral DEM for Pine Particle Physics

Tools

Developed XCT-informed polyhedral DEM for fundamental flow physics of fractured pine particles



Description

- Developed XCT-informed polyhedral DEM approach for study of the influence of particle morphologies (shape, size, etc.) and contact force models as CMAs in stress consolidation.

Value of new tool

- First-of-its-kind virtual laboratory for biomass particle mechanics.
- A fundamental and low-learning-curve design tool for industries.

Potential Customers & Outreach Plan

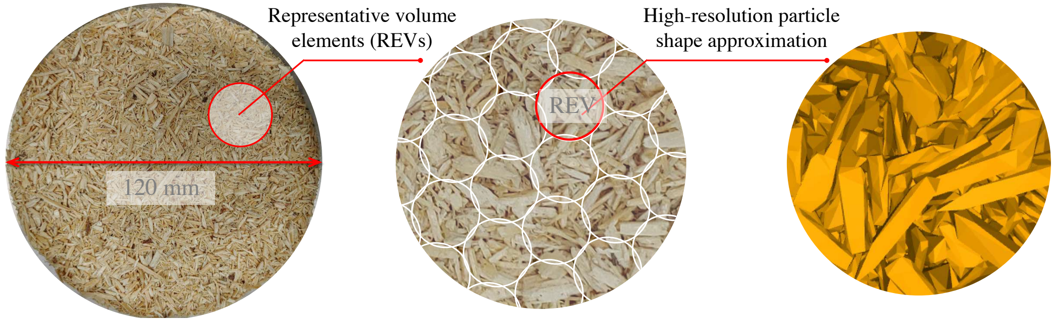
- Feedstock handling equipment suppliers, biorefinery designers.
- Bulk solids handling consulting & design companies.
- Academic communities for scientific studies.

Xia, Y. Chen, F., Klinger, J. Kane, J., Bhattacharjee, T., Seifert, R., Ajayi, O., Chen, Q. "Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation", *Biosystems Engineering*, 2021 (under review)

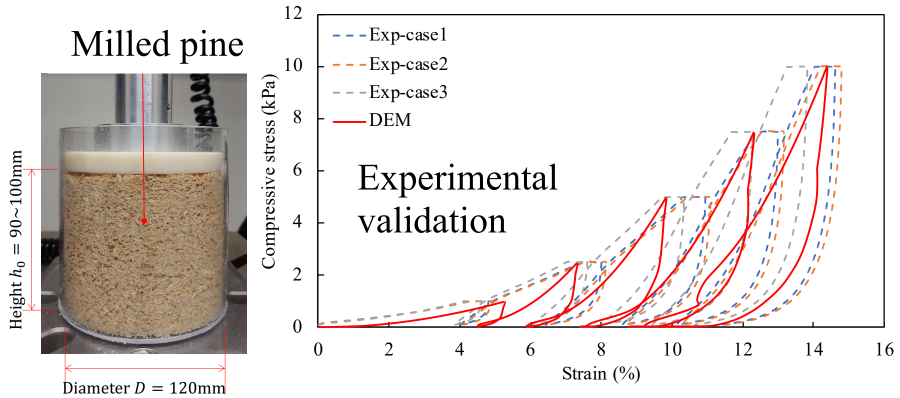
Coarse-grained DEM for Bulk Biomass Flow

Tools

Developed HPC-enabled open-source coarse-grain DEM for bulk biomass flow



A coarse-grained DEM with hysteretic nonlinear force-displacement contact laws



DOE HPCs enable determination of DEM biomass particle model parameters with 100,000 simulations in parallel!

Description

- An HPC-enabled open-source DEM package with low-cost, semi-empirical mechanistic contact laws.

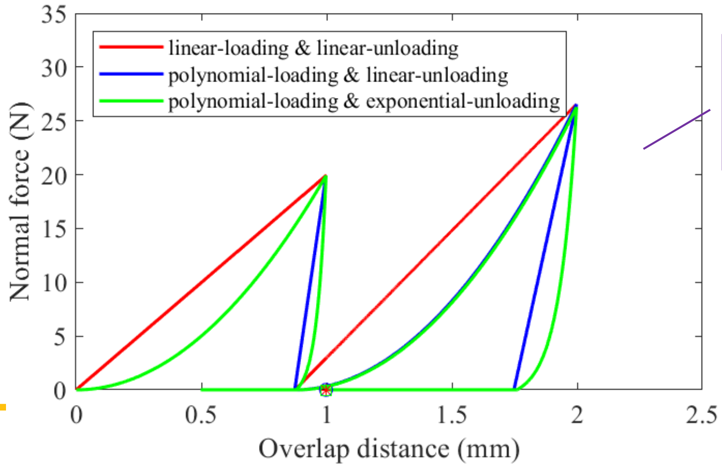
Value of new tool

- First-of-its-kind virtual laboratory for biomass particle mechanics.
- Open-source strategy maximizes flexibility of DEM development.
- A low-learning-curve design tool for industries.

forestconcepts™ bioenergy

Potential Customers & Outreach Plan

- Feedstock handling equipment suppliers, biorefinery designers.
- For academia as a fundamental scientific study tool.



--- Commercial DEM software
--- FCIC sponsored DEM codes
--- FCIC sponsored DEM codes

GitHub

Xia, Y. Chen, F., Klinger, Bhattacharjee, Chen, Q. "A nonlinear hysteretic contact model for the discrete element modeling of strain hardening of woody biomass", *Granular Matter*, 2021 (in preparation)

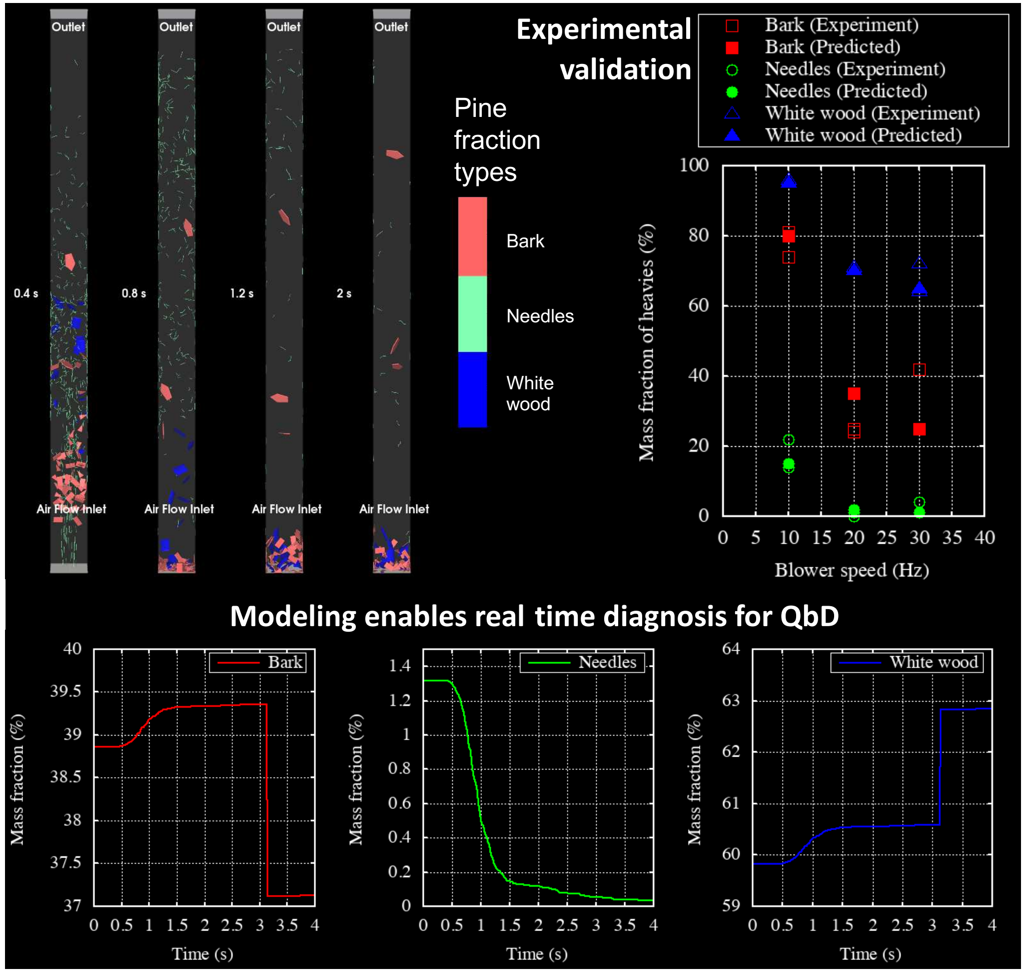
Print version

Material Handling x Preprocessing

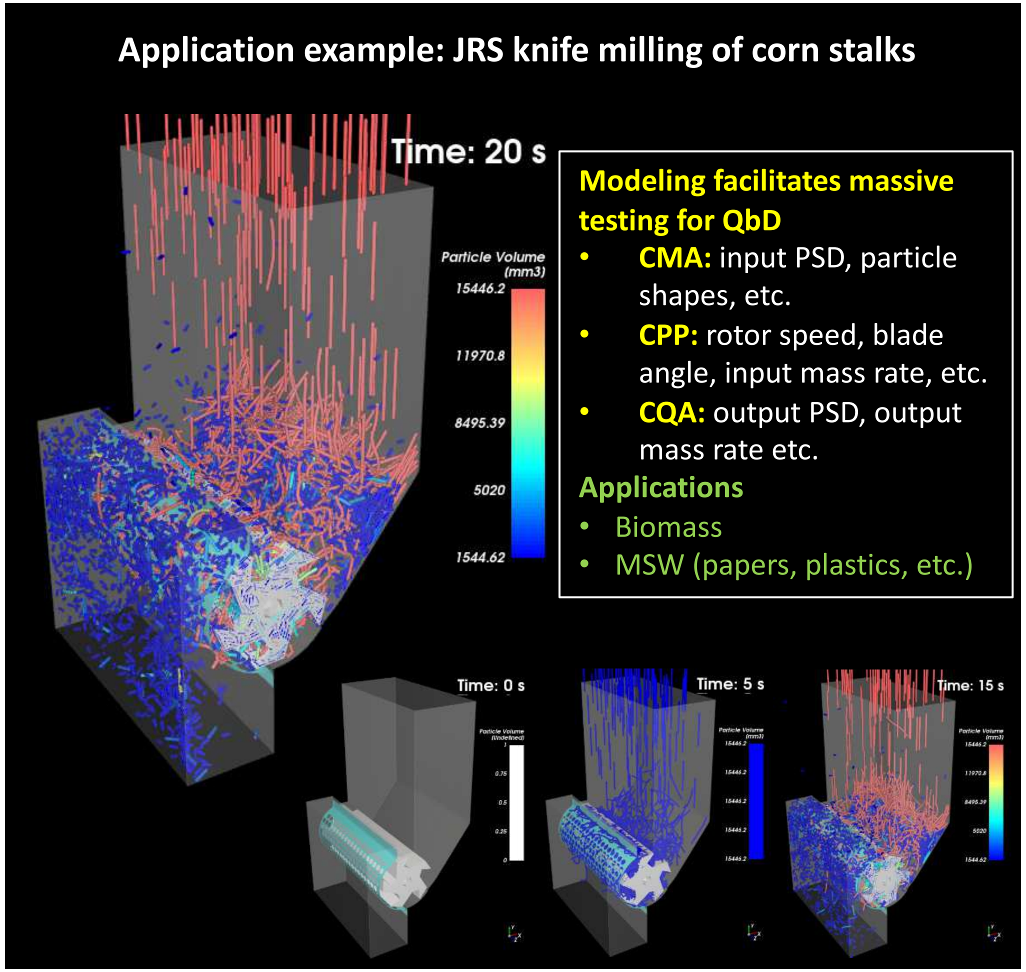
Crosscut: technique developed in Task 3 – Material Handling & applied to Task 5 – Preprocessing

Tools

Experiment-validated air-separation model



Experiment-informed knife-milling model



Description

- Supporting ***Quality-by-Design (QbD).***

Value of new tool

- First-of-its-kind virtual lab
- Fast testing and real-time diagnosis for design

Potential Customers & Outreach Plan

- Biorefinery
- Journals & Conference

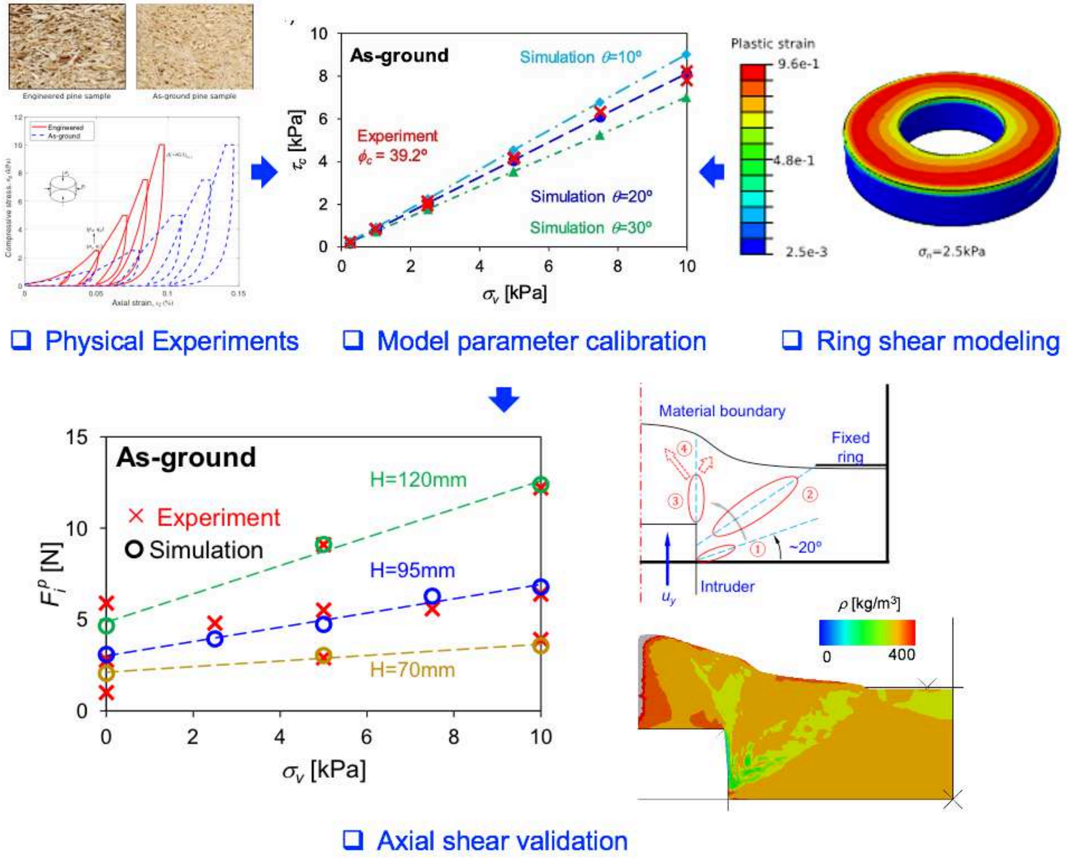
Print version

Continuum Flow Theories and Models

Knowledge

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Developed & validated advanced continuum particle flow theories & models to predict biomass in storage & slow flow conditions.



Current Knowledge Gap

- The state-of-the-art continuum flow models based on different theories and mathematical frameworks have not been evaluated for modeling biomass.
- Lab tests cannot provide direct measurement of constitutive model parameters due to the compressibility of particles

Achievement

- Established a work-flow to calibrate the model parameters by coupling standard laboratory tests with numerical simulations
- Implemented and evaluated four advanced continuum particle flow models for biomass granular material, and identified the hypoplastic model with critical state theory is the best one

Relevance

- Down-selection of a high-fidelity continuum flow model can better capture the biomass flow physics, which will used to design equipment for academia and industrial stakeholders.

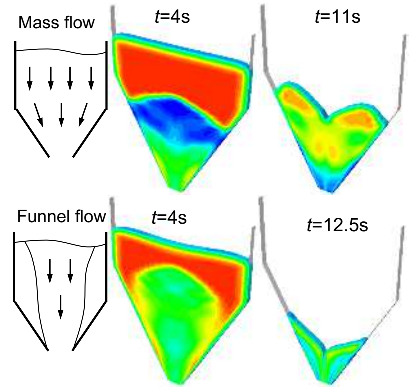
A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine, *Powder Technology*, 368:45-58, 2020. https://doi.org/10.1016/j.powtec.2020.04.038

Print version

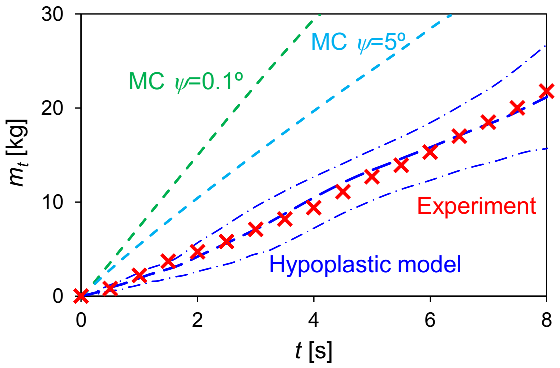
Continuum Model for Flow Design Guidance

Tools

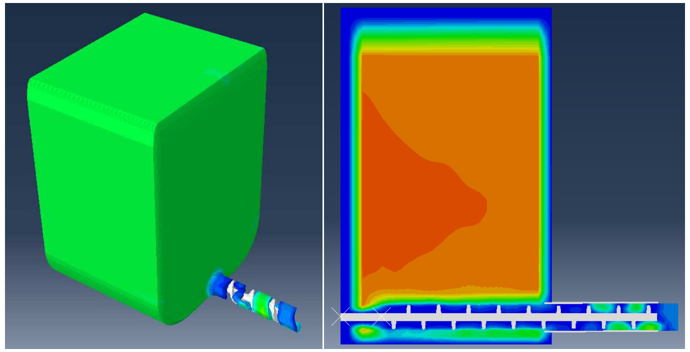
Used reformulated continuum particle flow models to predict biomass & guide design of pilot-/industrial-scale hopper & conveyor.



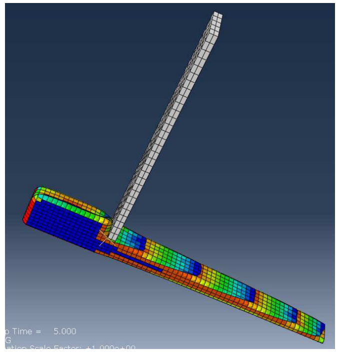
❑ Hopper flow pattern prediction



❑ Quantitative flow rate validation



Engineering Application - modeling Acrison feeding system



❑ Inclined plate flow modeling

This work is performed jointly with the "Bio-crude Production and Upgrading to Renewable Diesel"

Description

- Validated the hypoplastic model to accurately capture the flow behavior in a pilot-scale hopper, applied the model to capture flow behavior in the Acrison feeder at industrial-scale

Value of new tool

- 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

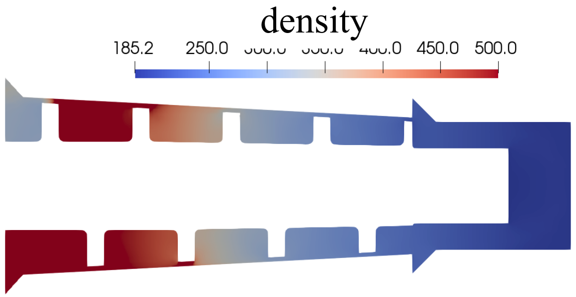
- Biomass feedstock handling equipment suppliers, biorefineries
- Academic communities for scientific studies
- Open-source continuum mechanics models for general public

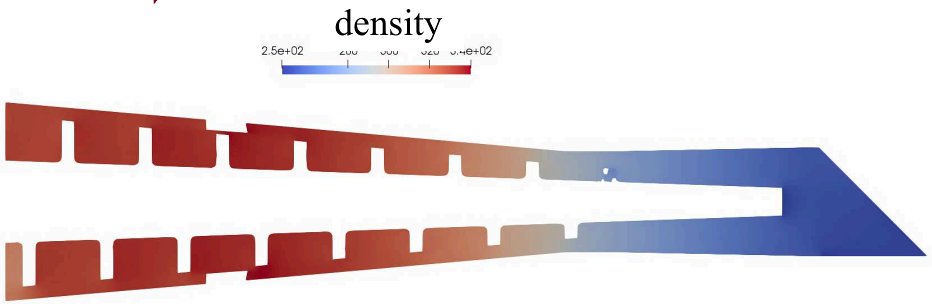
Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model, Powder Technology (2021).

CFD Model of Compression-Screw Feeders

Tools

Computational fluid dynamics (CFD) model developed for the dynamic flow of milled lignocellulosic biomass in compression-screw feeders





This work was performed jointly between the FCIC and a competitively awarded project, “Integrated Computational Tools to Optimize and De-Risk Feedstock Handling & High- Pressure Reactor Feedings Systems,”

Description

- Experiment-based novel models are necessary for resolving the deformation behavior of the biomass material
- Simulated torque of wood chips or corn stover being compressed and transported through pilot-scale feeders quantitatively agreed with experimental measurements.

Value of new tool

- Engineering calculation dependent design and operation of compression-screw feeders poorly predicts process upsets
- The CFD models can be used to evaluate feeder performance for different operating conditions and to study upset dynamics.

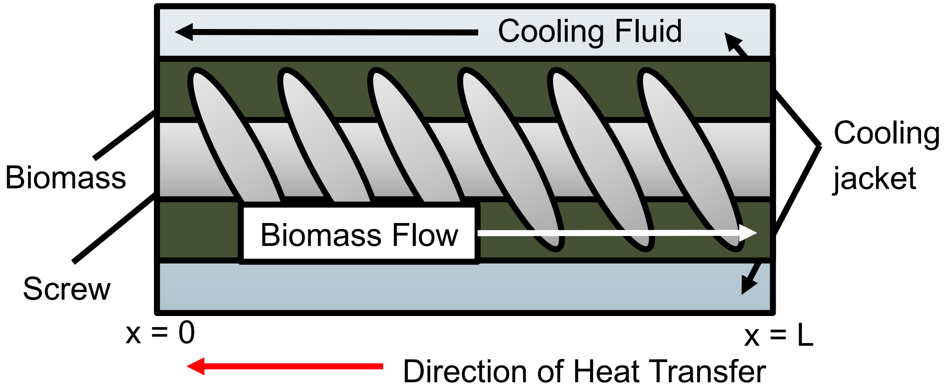
Potential Customers & Outreach Plan

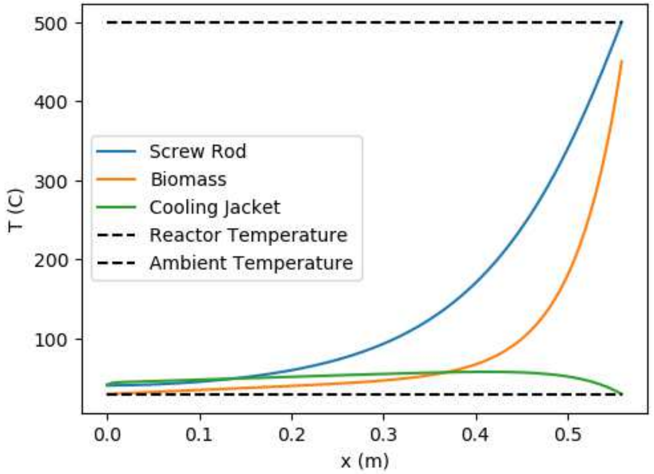
- Biomass feeding-equipment suppliers and biorefinery designers
- Models made available via open-source models offered for public use and CRADA projects between industry and labs to enable simulations on HPC

Temperature Modeling of Pyrolysis Feeder

Tools

1D convection and heat transfer models predict the temperature of biomass in pyrolysis screw-auger feeders





Description

- Elevated temperatures can result in premature reaction and plugging of the feeder, as has been observed in NREL's 2FBR pyrolysis-reactor system
- Coupled 1D temperature models of each component in the feeder system provide a low-fidelity but computationally efficient prediction of biomass temperature.

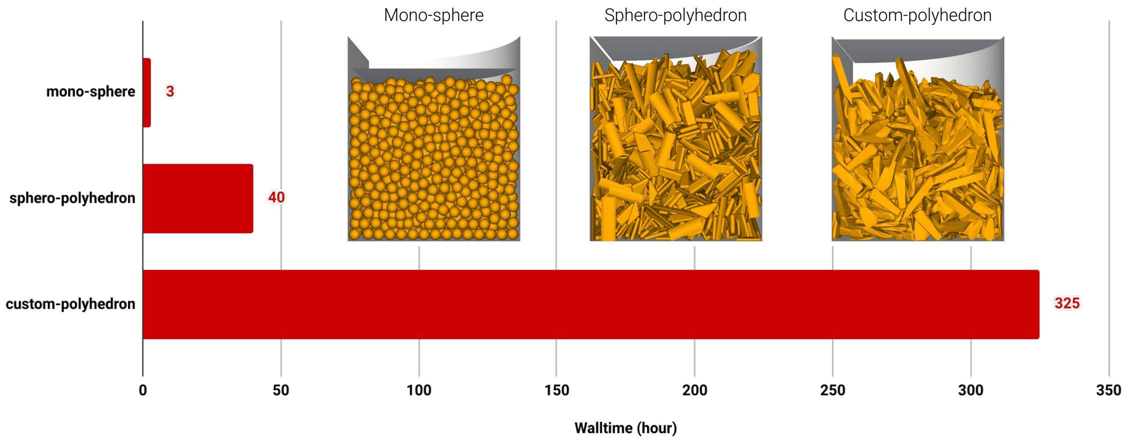
Value of new tool

- Model predictions can suggest feeder designs and operating conditions that improve the biomass temperature profile.

Potential Customers & Outreach Plan

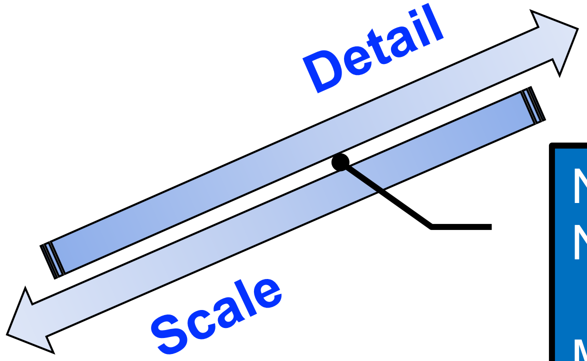
- Model was made available to NREL engineers via a Jupyter notebook (simple GUI).
- Notebook will be shared publicly via GitHub repository after the model is validated against feeder temperature measurements.

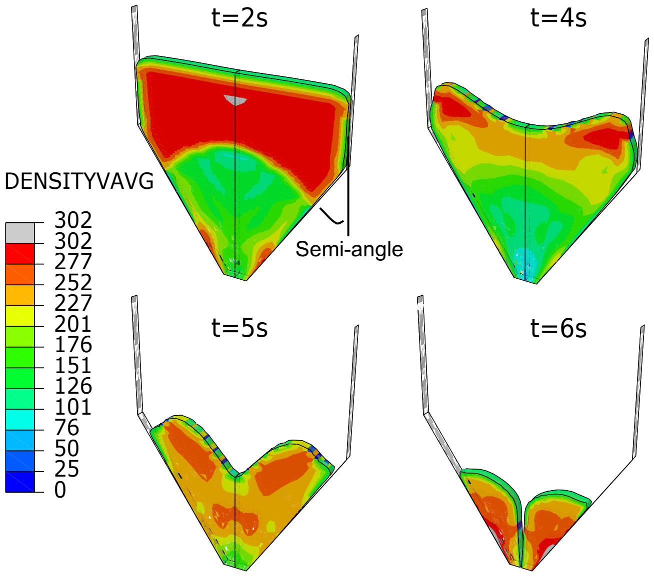
What Flow Models to Choose?



DEM particle axial shear simulation:

- Size: ~50mm (~2000 particles)
- Resource: 4 CPU cores
- Cost: **300 hours** with polyhedral DEM model
- Cost: **3 hours with** coarse-grained DEM model





FEM pilot-scale hopper simulation
[Jin et al, 2020]:

- Size: ~1000mm;
- Resource: 32 CPU cores
- **Cost: 2 hours**

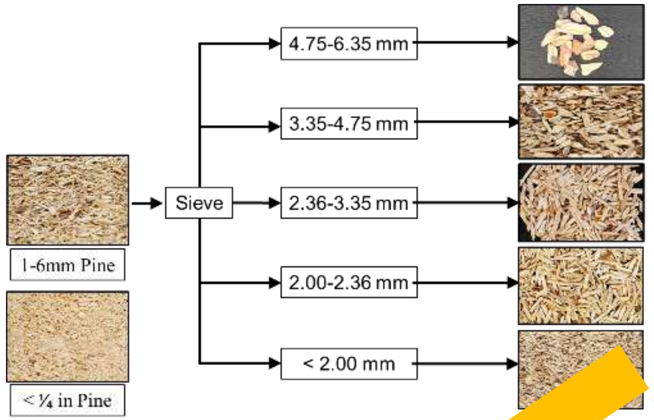
No access to HPC?
Not a problem.

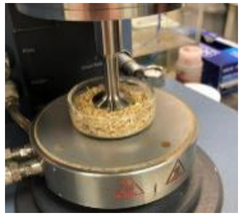
Most simulations shown here require only a good personal workstation to complete within a reasonable amount of time.

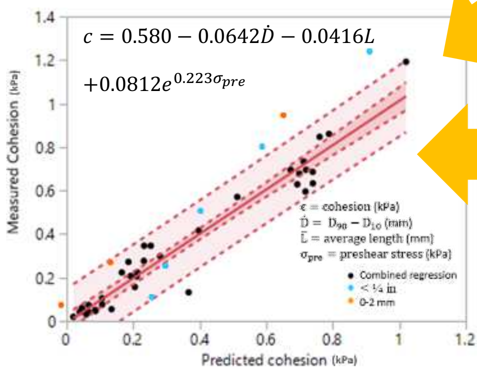
Multiscale Bulk Flow Characterization

Knowledge

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







Current Knowledge Gap

- Current state-of-the-art granular characterization methods and models developed for incompressible, regular solids.
- These methods cannot be applied directly to biomass because of anisotropic compressibility, bulk creep, and heterogeneity/variability.
- Current quasi-static test methods / properties do not directly predict flow performance in pilot equipment such as has been developed for powders and soils.

Achievement

- Develop multiscale characterization methods and pair with validation data to correlate material attributes with bulk flow performance (such as flow inception and critical state shear properties)

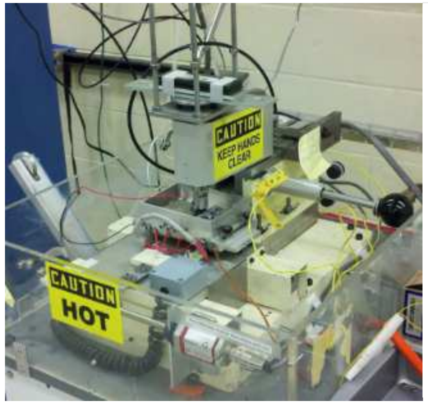
Relevance

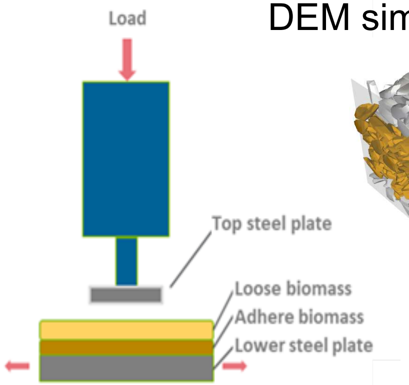
- Understanding how characterization methods and material properties impact flow performance will allow for better materials characterization by academia and industrial stakeholders, as well as more robust testing and equipment design for bioenergy feedstocks.

Particle Friction Measurement

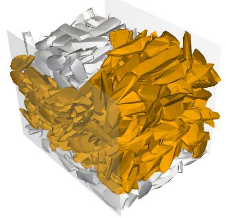
Knowledge

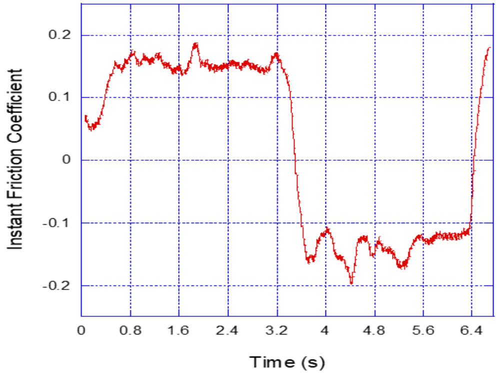
Adapted high precision tribometer to measure the instantaneous particle-particle and particle-wall friction of biomass materials.

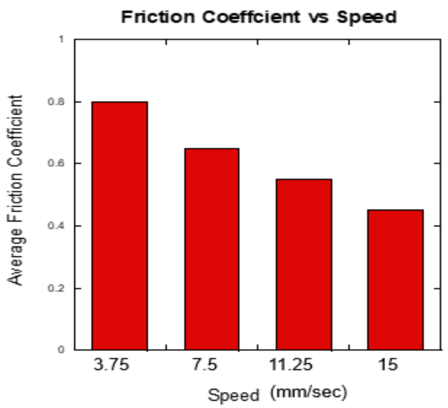




DEM simulation







Current Knowledge Gap

- Current practice extracts average friction from shear tests.
- Inadequately for detailed understanding of friction behavior.

Achievement

- Adapted high precision tribometer to accurately measure instantaneous particle-particle friction and particle-wall friction. Average friction can also be calculated.
- Determined effect of load (pressure), speed (shear rate), RH, particle size on friction behavior of pine particles.

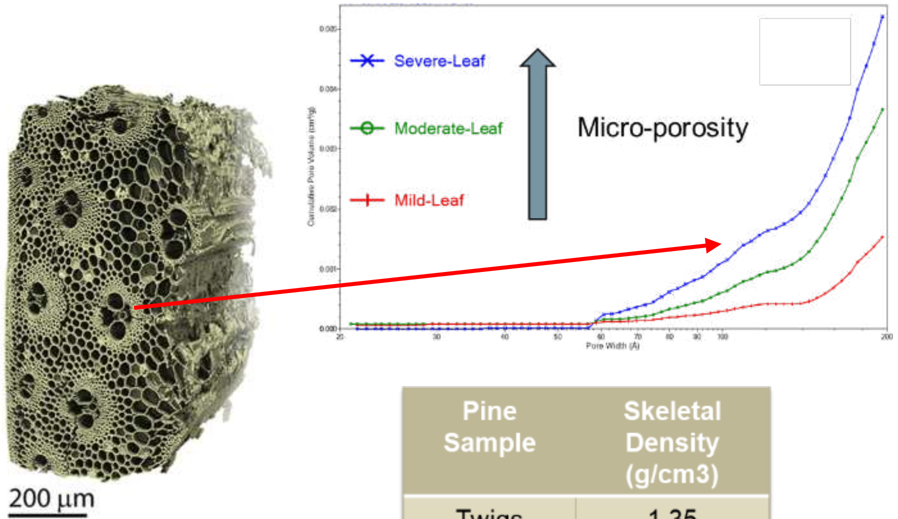
Relevance

- The data provide input for DEM modeling of biomass material.
- The basic physics of mechanisms of friction in biomass materials can be extracted from frictional behavior measurements.
- Eventually, the data can enable formulation of constitutive equation for friction behavior of biomass materials.

Measuring Porosity, Pore Volume, & Density

Knowledge

Advanced gas pycnometry and mercury intrusion porosimetry to quantify porosity and density



Ciesielski, et. al "Advances in Multiscale Modeling of Lignocellulosic Biomass." *ACS Sustainable Chemistry and Engineering*. **2020**

Pine Sample	Skeletal Density (g/cm3)
Twigs	1.35
Bark	1.39
Needles	1.75

Current Knowledge Gap

- Accurate measurements for density, porosity & pore volume for anatomical fractions of corn stover and loblolly pine
- How density, porosity & pore volumes change as a function of storage, harvesting operation, pretreatment, and age

Achievement

- Quantified the variability in corn stover, loblolly pine, and anatomical fractions
- Quantified the variability resulting from biological degradation, storage and pretreatment. Microporosity increases with degree of biological degradation.
- Identified porosity, pore volume, density and surface area as critical material attributes for modeling and/or pretreatment

Relevance

- Data are direct inputs for DEM & reactive transport models.
- Develop LAPs for data across global community to develop consistent data sets for data mining, TEA/LCA, & modeling.

Summary

Management:

The Task-3 Material Handling team has 1) fulfilled project milestones, 2) disseminated continual research excellence, and 3) established collaboration with relevant industry and academia, via management strategies including: 1) timely communication (between labs and with DOE & industries), 2) adaptive market identification (for open-source software & CRADAs), and 3) synergistic R&D (between labs and with universities in FOAs).

Technical Approach:

This task has established an integrated multiscale experimental and physics-based modeling approach for the R&D of first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat.

Impact:

This task will provide biomass industry with suitable & predictive design tools to effectively assist design of feedstock processing & handling equipment, including design charts and open-source flow model packages.

Progress:

This task has delivered all the milestones & technical achievement to date, published articles & proceedings in high-impact-factor journals and conferences, and attained growing market impact in the biomass industry.

Quad Chart Overview- FCIC, Task 3 – Material Handling

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Timeline

- 10/1/2018 - 9/30/2021

	FY20	Active Project
DOE Funding	$1,874,000	FY19- $2,200,000 FY20- $1,874,000 FY21- $1,885,000 Total- $5,953,000

Project Partners (N/A)

Barriers addressed

Major

- Operational Reliability (19Ft-J, FSL)
- Materials Compatibility, and Equipment Design and Optimization (19ADO-H, ADO)

Supporting

- Feedstock Quality: Monitoring and Impact on Preprocessing and Conversion Performance (19Ft-E, FSL)

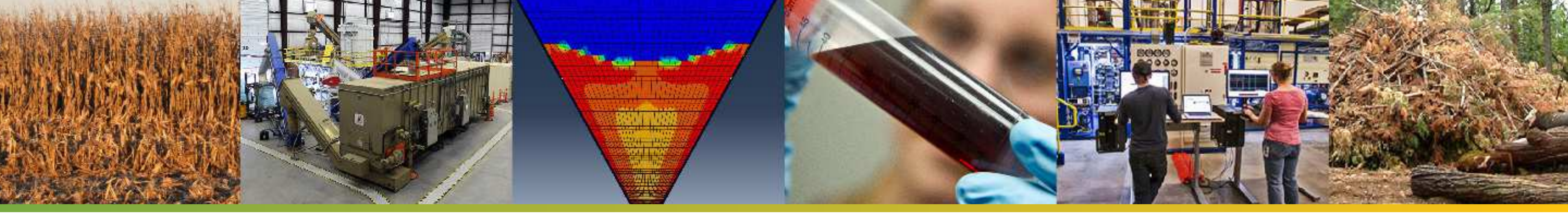
Project Goal

The project goal of Task-3 Material Handling is to develop first-principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat.

End of Project Milestone

Completion of the experimental measurement and simulation data needed for the draft design chart document of industrial-relevant wedge-shaped hopper (INL) and conical hopper (NREL), including the semi-angles, wall friction angles, and outlet sizes predicted by industry-scale simulation using calibrated flow models.

Funding Mechanism (N/A)



Thank you

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INTERFACE CONSORTIUM

Responses to Previous Reviewers' Comments

From the predecessor project "Feedstock Physical Performance Modeling"

Comment: The early cellulosic biorefineries experienced significant problems in the interface of feedstock handling and conversion. The modeling created in this project suggests that if a project developer understands the physical properties of the feedstock in their plan, the proper feeding and handling system could be designed and hopefully not have the same sorts of problems that the industry presently faces. This could be an important step forward in the SOT as it exists today.

Response: Agreed. The advanced simulation and characterization methods will enable consulting firms in bulk solids handling to properly advise industrial biorefineries, and the rapid and reduced-order models will be directly useful for industrial biorefineries to better understand the effects of feedstock variability.

Responses to Previous Reviewers' Comments

<u>From the predecessor project "Feedstock Physical Performance Modeling" (continued)</u>

Comment: This project undertook a very challenging application, and, not surprisingly, it found that several models need to be applied simultaneously to get reasonable system models. Congratulations on the frontier-type work; the reviewer anticipates that it will lead to new concepts for improving biomass flow through hoppers and screws.

Response: Exactly. It is also understood that the project developer will likely need to consult with firms that specialize in handling bulk solid (particulate) materials to appropriately apply advanced methods developed by this project.

Responses to Previous Reviewers' Comments

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

From the predecessor project "Feedstock Physical Performance Modeling" (continued)

Comment: Relevant industry partners were involved in the project, but it was not clear where they had vetted the modeling analysis or this had been done only on the flow characterization methods. The reviewer suggests this is done as part of fully completing the work and helping to ensure its value to equipment designers.

Response: Industry partners primarily assisted by helping with the flow characterization methods and early discussion of simulation options. As the models develop and additional results are obtained, input will be sought from a wide range of industry and academic experts. This input will be sought through subcontracts and through the Particle Technology Forum within the American Institute of Chemical Engineers.

Responses to Previous Reviewers' Comments

<u>From the predecessor project "Feedstock Physical Performance Modeling" (continued)</u>

Comment: A variety of flow modeling methods were applied, although the details were difficult to follow. This is an interesting project, but a model with a goal of an R-square of 0.8 might not be able to drive significant improvements. The results of the project are of limited impact on the overall biorefining industry. This is because a new set of tests would likely be required depending on the equipment and feedstock used. Unfortunately, the calculation approach failed to provide usable results.

Response: We agree that being able to predict flow behavior with 80% accuracy might not be adequate for the industry. Current advanced models that we have tested exhibit errors that are greater than 100% for key multidimensional predictions. We believe that the models can be improved substantially, which will lead to improved understanding and more reliable designs. Efforts at adapting advanced continuum and particle models are still in their relative infancy and will be pursued further in a future project to provide useful results.

Publications, Patents, Presentations, Awards, and Commercialization

Peer-reviewed journal articles (including manuscripts under review and in revision)

- Cheng, Z., Leal, J., Hartford, C., Carson, J., Donohoe, B., Craig, D., Xia, Y., Daniel, R., Ajayi, O., Semelsberger, T. “Flow behavior characterization of biomass feedstocks”, *Powder Technology*, 2021 (under review).
- Xia, Y. Chen, F., Klinger, J. Kane, J., Bhattacharjee, T., Seifert, R., Ajayi, O., Chen, Q. “Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation”, *Biosystems Engineering*, 2021 (under review)
- Jin, W. et al. “Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model”, *Powder Technology*, 2021.
- Jin, W., Klinger, J. Westover, T. and Huang, H. “A density dependent drucker-prager/cap model for ring shear simulation of ground loblolly pine: advantages and limitations”. *Powder Technology*, Vol. 368, pp. 45-58, 2020
- Xia, Y., Stickel, J., Jin, W., Klinger, J. “A review of computational models for the flow of milled biomass I: Discrete-particle models”. *ACS Sustainable Chemistry & Engineering*, 2020, 8, 16, pp. 6142-6156
- Jin, W., Stickel, J., Xia, Y., Klinger, J. “A review of computational models for the flow of milled biomass II: Continuum-mechanics models”. *ACS Sustainable Chemistry & Engineering*, 2020, 8, 16, pp. 6157-6172
- Guo, Y., Chen, Q., Xia, Y., Westover, T., Eksioglu, S. Roni, M. “Discrete element modeling of switchgrass particles under compression and rotational shear”. *Biomass & Bioenergy*, 2020
- Xia, Y., Lai, Z., Westover, T., Klinger, J., Huang, H., Chen, Q. “Discrete element modeling of deformable pinewood chips in cyclic loading test”, *Powder Technology*, Vol 345, 1, pp. 1-14, 2019.

Publications, Patents, Presentations, Awards, and Commercialization (continued)

Presentations at professional conferences (FY20 – FY21)

FCIC Webinar series

- Xia, Y. & Ciesielski, P. "FCIC Modeling 1", February 11, 2021.

2020 Virtual AIChE Annual Meeting, November 16-20, 2020

- Rahimi, M. et al. "Computational modeling of a biomass screw-feeder with compressible non-Newtonian rheology".
- Chen, F. et al. "A Hysteretic Nonlinear Elastoplastic Contact Model for Discrete Element Modeling of Milled Woody Biomass".
- Jin, W. et al. "A Multi-Regime Continuum Approach for Modeling Flow of Granular Pine Chip".
- Jin, W. et al. "Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine".
- Ahsan, S. et al. "Computational Fluid-Dynamics Modeling of Biomass-Feedstock Flow Using a Non-Local Granular-Fluidity Constitutive Model".
- Bhattacharjee, T. et al. "Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine".

International Powder & Bulk Solids Conference & Exhibition, The Powder Show Digital Flow (virtual), October 1, 2020.

- Xia, Y. "Limitations and Best Practice for DEM Modeling of Biomass".

ASABE Annual Meeting 2020 (virtual), July 13-15, 2020

- Xia, Y. et al. "FCIC Materials Handling Project Overview and R&D Highlights".
- Klinger, J. et al. "Bulk Physical, Mechanical, and Shear Properties of Loblolly Pine and Flow Characterization in Variable Wedge Hopper Geometries".
- Jin, W. et al. "Multi-scale Computational Modeling of Milled Biomass Flow with Multi-regime Constitutive Model".
- Xia, Y. et al. "Discrete Element Modeling for the Flow of Milled Biomass: Current State of the Art and Applications".
- Ahsan, S. et al. "Non-local granular fluidity based constitutive modeling of woody biomass feed flow".

Publications, Patents, Presentations, Awards, and Commercialization (continued)

Presentations at professional conferences (FY19 – FY20)

2019 AIChE Annual Meeting, November 10-15, 2019, Orlando, FL.

- Jordan, K. et al. "Experimental Study of Intermediate Storage and Discharge of Compressible Biomass Particulate Solids in a Wedge-Shaped Hopper of Changing Geometry".
- Bhattacharjee, T. et al. "Mechanical Properties and Bulk Flow Characterization of Loblolly Pine."
- Xia, Y. "Discrete Element Modeling of Granular Flow of Flexible Woody Biomass Particles".

2019 The Society of Rheology Annual Meeting

- Stickel J. et al. "Parameter determination of the non-local granular fluidity model for wood chips by comparison to well-defined experimental flow systems."

Engineering Mechanics Institute Conference 2019, June 18-21, 2019, Pasadena, CA.

- Xia, Y. et al. "Discrete Element Modeling of Granular Flow of Flexible Woody Biomass Particles".
- Jin, W. et al. "On the Implementation and Application of a Critical State Particle Mechanics Enhanced Drucker-Prager/Cap Model for Biomass Flow".

2019 AIChE Annual Meeting, October 28 – November 2, 2018, Pittsburg, PA.

- Westover, T. et al. "Flow Behavior of Particulate Pine Forest Residues and Corn Stover: A Comparison of Experiments and Simulations".

Publications, Patents, Presentations, Awards, and Commercialization (continued)

Awards

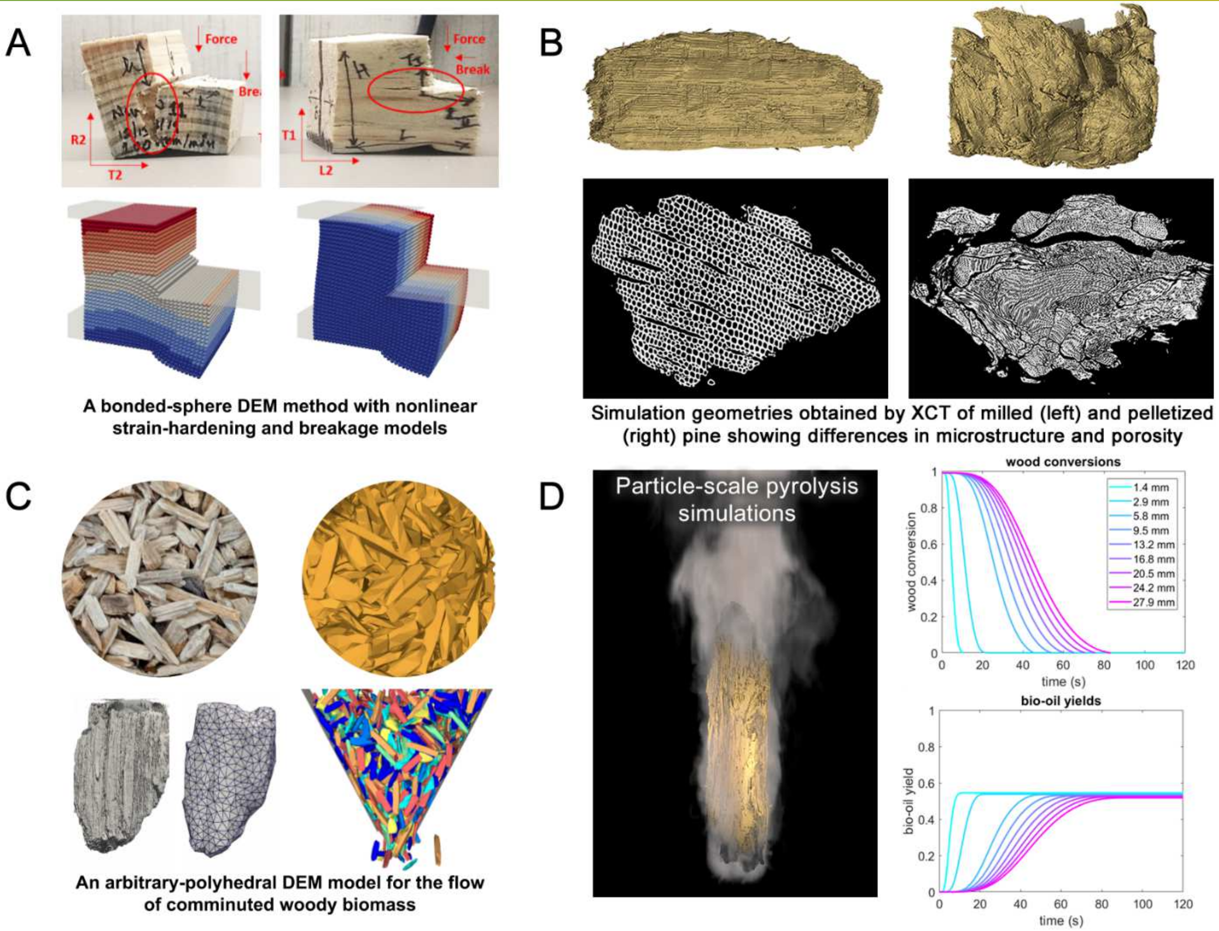
Best Poster Award @ 2020 Virtual AIChE Annual Meeting, November 16-20, 2020.

Bhattacharjee, T. et al. “Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine”.

Best Poster Award @ 2019 AIChE Annual Meeting, November 10-15, 2019, Orlando, FL.

Bhattacharjee, T. et al. “Mechanical Properties and Bulk Flow Characterization of Loblolly Pine.”

Publications, Patents, Presentations, Awards, and Commercialization (continued)



CCPC/FCIC simulation methods that will be leveraged by this project. (A) DEM fragmentation models. (B) Microstructured particle geometries from XCT reconstructions. (C) Flowability simulations using realistic particle geometries. (D) Thermochemical conversion simulations accounting for detailed particle attributes.

A project "***Quantifying Improvements in Feedstock Performance Resulting from Forest Concepts'*** *Preprocessing Technology*" proposed by Forest Concepts, LLC, of Auburn, Washington in partnership with **NREL** and **INL** is among the three projects that received **DOE DFO award** via the DOE BETO CCPC (in partnership with FCIC). By incorporating high-performance computing, researchers can help reduce the costs and time needed for conversion process scale-up and reactor design. In the awarded DFO project, Forest Concepts will work with INL and NREL to model the behaviors of different biomass types undergoing Forest Concepts' preprocessing technologies as well as the downstream conversion effects.

Relevant FCIC Tasks

- Task 3 Material Handling
- Task 5 Preprocessing
- Task 6 High Temperature Conversion

CCPC Consortium for Computational Physics and Chemistry
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