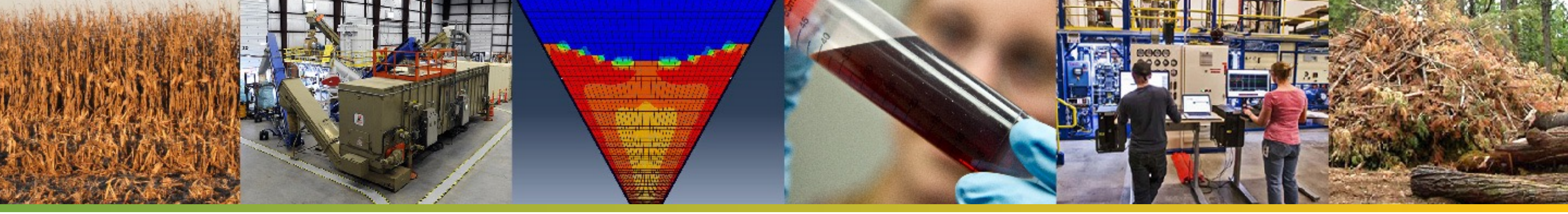
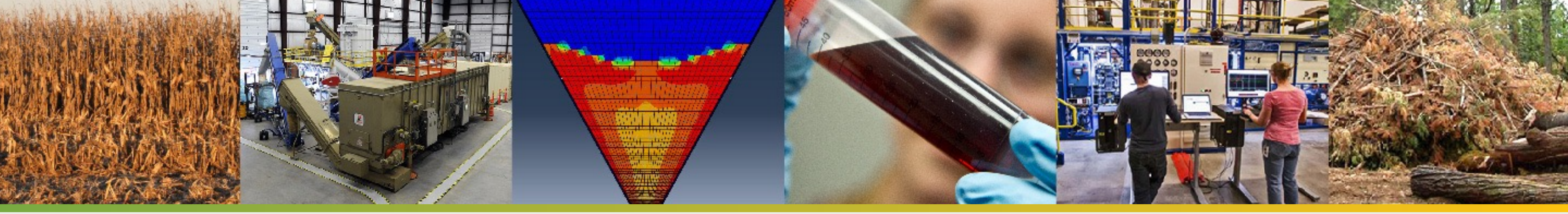


DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

FCIC Task 3 – Material Handling

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

Yidong Xia
Idaho National Laboratory



Project Overview

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

FCIC Task Organization

Feedstock | Preprocessing | Conversion

Task 2: Feedstock Variability

Task 5: Preprocessing

Task 6: High-Temperature Conversion

Task 7: Low-Temperature Conversion

Task 1: Materials of Construction

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 & 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

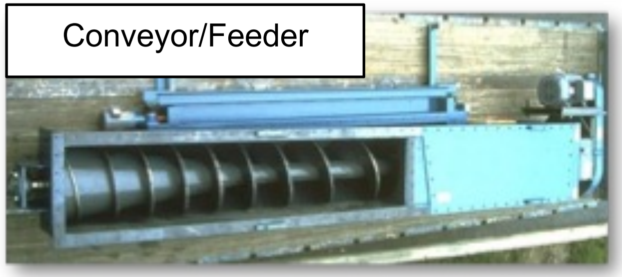
Task 6 & 7: Conversion (High- & Low-Temp Pathways): Produce intermediates for further processing

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

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

Project Overview – Motivation

Process upsets



BETO "Biorefinery Optimization Workshop Summary Report", 2016. [URL]

A **primary challenge** in the design of a biorefinery is the storage, transport, and reactor feeding of the biomass feedstocks.

Material handling/feeding is prone to process upsets such as jamming and clogging, resulting in increased downtime and ultimately higher costs.

Commercial-scale conversion of biomass in **biorefineries** remains limited.

Project Overview – Objective

Objective:

- Develop **first principles-based design tools** that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat and enable applications of the developed tools to industry stakeholders.

Impact:

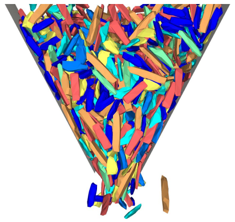
- **Reliable working envelopes of CMAs and CPPs for CQAs of operation units**, e.g., design charts for consistent flow. Validated design tools (design charts, open-source flow simulation codes) for equipment designers.
- QbD-based predictive design paradigms & tools for industry to effectively assist their design of feedstock processing & handling equipment

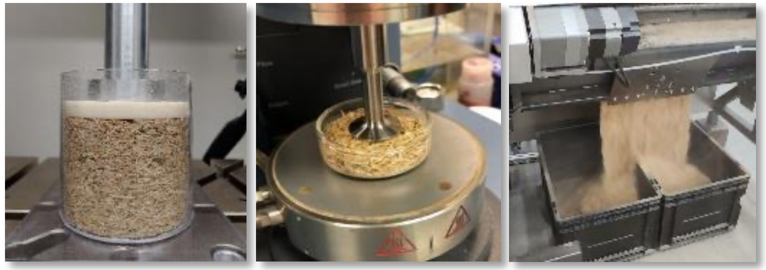
Outcome:

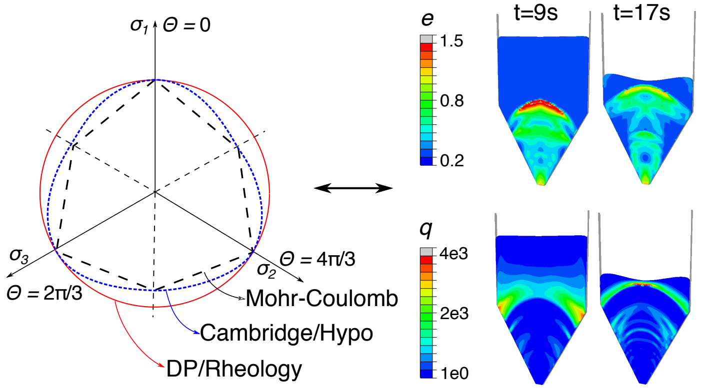
- **Open-source feedstock flow simulation tools** for multiple scales.
- **Reliable feeding and handling solutions** achieved through physics-based, experiment-informed & validated modeling tools and measurement.


Chipped loblolly pine particles


Polyhedral particles of arbitrary shapes


A v-shape hopper discharge simulation





Task 3 Quality-by-Design (QbD) Summary

Unit Operation	Critical Material Attribute (CMA)	Critical Processing Parameter (CPP)	Critical Quality Attribute (CQA)
Wedge hopper	Bulk scale ↕ Multiscale ↕ Particle scale Bulk critical-state density; Bulk critical-state friction angle; Bulk-wall friction angle Bulk dense flow friction angle; Bulk elasticity. Surface energy; Moisture content; Ash content; Particle size distribution (PSD); Particle shape aspect ratio (L/W); Particle density (envelope); Particle porosity (envelope); Particle elasticity (dense).	Outlet width; Wall inclination angle; Feeding mass rate	Discharge mass rate; Critical arching distance.
Screw conveyor		Shaft rotation speed; Pitch (blade spacing / diameter; Feeding mass rate	Output mass rate; Torque at jamming.

The Material Handling Team: Collaborating across Four Labs

Idaho National Laboratory


Wencheng Jin
Ph.D.


Yidong Xia
Ph.D.


Jordan Klinger
Ph.D.


Tiasha Bhattacharjee


Nepu Saha
Ph.D.


Ahmed Hamed
Ph.D.

Argonne National Laboratory


Oyelayo O. Ajayi
Ph.D.

NREL – National Renewable Energy Laboratory


Hariswaran Sitaraman
Ph.D.


Jonathan Stickel
Ph.D.
(Previous member)


Yudong Li
Ph.D.


Syed Ahsan
Ph.D.
(Previous member)

Los Alamos National Laboratory

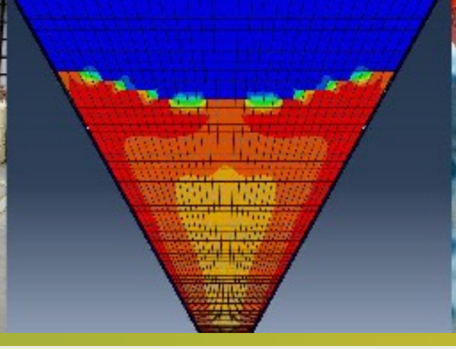

Benjamin Davis
Ph.D.


Troy Semelsberger
Ph.D.
(Previous member)


Ricardo Navar
Ph.D.


(Lily) Ziwei Cheng
Ph.D.
(Previous member)






1 – Approach

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

U.S. DEPARTMENT OF ENERGY

1 – Approach

Technical Approach: An integrated multiscale experimental and physics-based modeling approach

Experimental:

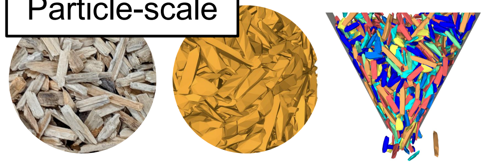
Particle-scale

Bulk-scale

Pilot/demonstration-scale

Computational:

Particle-scale

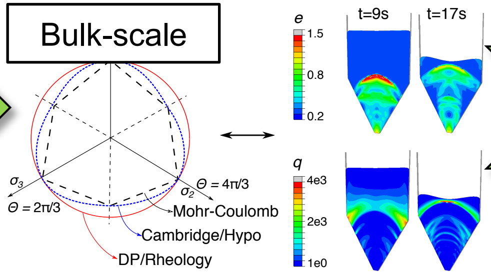


Chipped loblolly pine particles

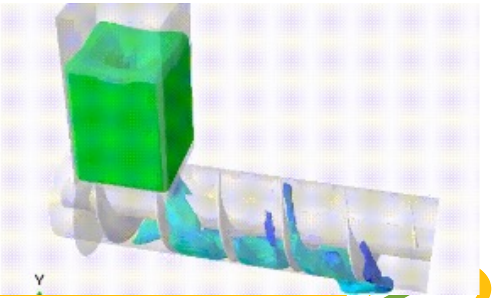
Polyhedral particles of arbitrary shapes

A v-shape hopper discharge simulation

Bulk-scale



Pilot/demonstration-scale



Outcome: Design charts & open-source modeling toolkits

Preprocessing

CQA (particle size, feed rate, etc.)

CMA & CPP (particle size, feed rate, etc.)

Material Handling

CQAs (flow rate)

CMA & CPP (particle size, feed rate, etc.)

Conversion CQAs

GTI ENERGY

forestconcepts bioenergy

BHS BulkHandling SYSTEMS

advancebio Fuel & Chemical Technologies

1 – Approach

Technical Approach

- An integrated multiscale experimental and physics-based modeling approach.

Challenges

- How to adapt experimental design to meet industry stakeholders' priority and maximize impact.
- How to de-risk uncertainties in the predictability & robustness of the developed computational models.

Metrics

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

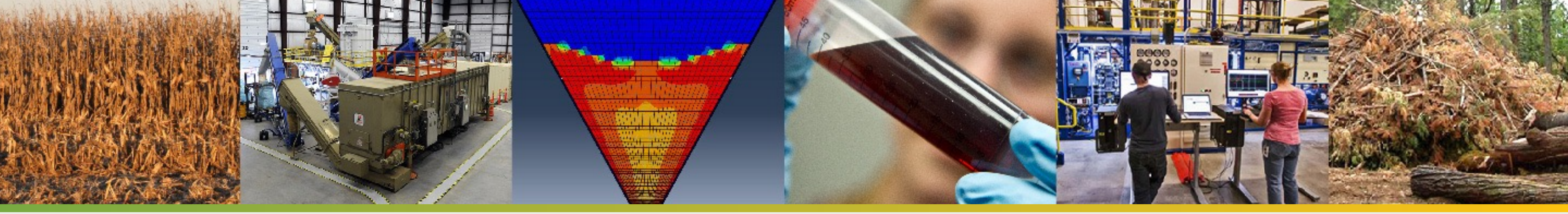
Risks/Mitigation Strategies

- Risk: Lack of synergy between experimentalists and modelers, between lab scope and industry priorities.
- Mitigation: Involve modelers in experimental design & testing; engage in communication with stakeholders.

Communication/Collaboration

- Two task meetings per month and cross-task meetings. Members involved in industry collaboration projects.
- Conference presentations at AIChE, ASABE, and International Biomass Conference & Expo.

DEI – Hired and supported female ethnic minority student intern and career development



2 – Progress and Outcomes

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Roadmap & Outline of Progress

EXPERIMENTAL WORK

Multiscale flowability test for milled pine particles → Pilot-scale handling operation test for milled pine particles

Data, validation, and best practice

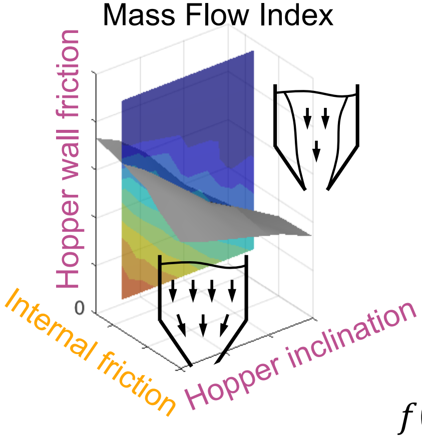
Data, validation, and extended predictions

MODELING WORK

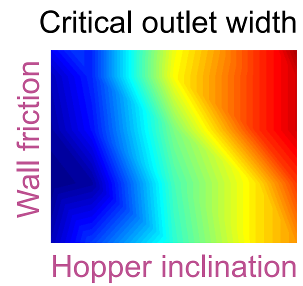
Micro- to macro-scopic flow models for granular biomass → Pilot-scale handling modeling for milled pine particles

Hopper design charts for milled pine particles

Mass Vs. Funnel flow



Hopper arching



Flow throughput

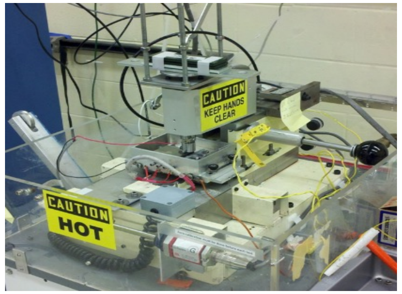
$f(\rho_p, d_{50}, \phi_c, L, W, \mu) = \text{Mass flow rate}$

Material attributes **Hopper parameters**

Multiscale Characterization Suite for Flowability of Granular Biomass and MSW

Tools

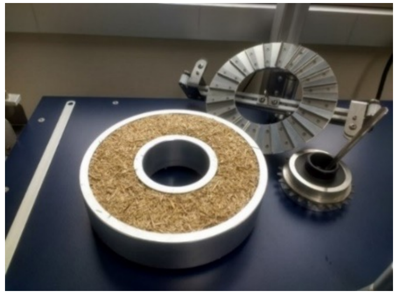
Particle scale → **Pre-pilot scale** → **Pilot scale**



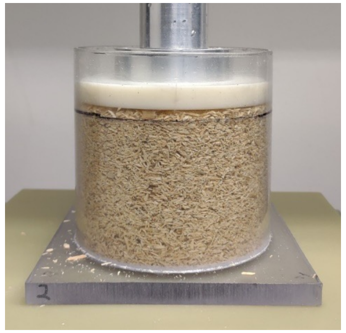
(ANL) Reciprocating tribometer

(LANL) Powder rheometer

(INL) Density analyzer



(INL) Ring shear



(INL) Axial load cell

(INL) Inclined plane flow tester

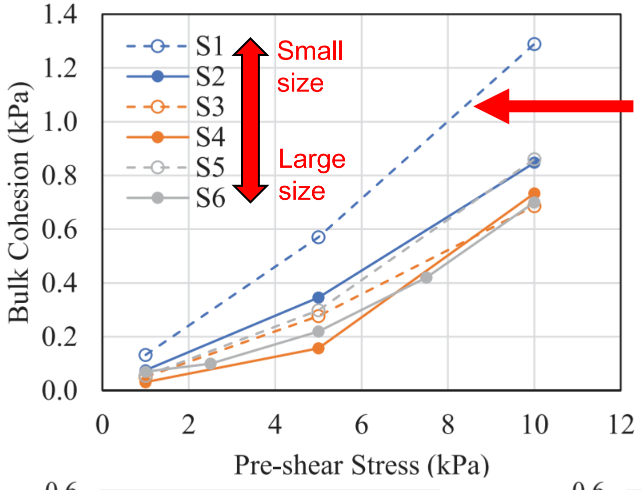
(INL) Adjustable flow hopper

(INL) Screw feeder for testing mechanically driven flow

Multiscale Correlations from Particle Size & Distribution to Flowability of Milled Pine

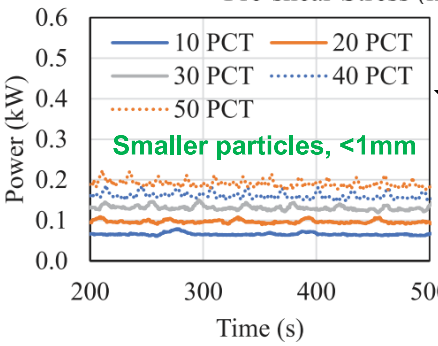
Knowledge

Influence of particle size & distribution on shear and flow properties: Smaller particles leads to more consistent, and lower power draw from screw conveyors.

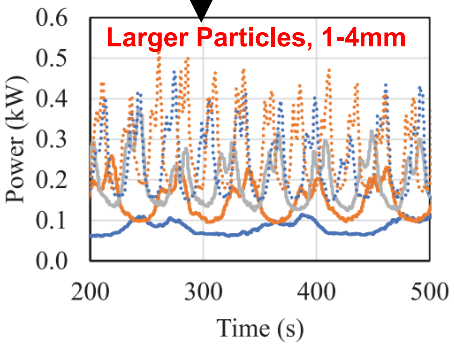


Smaller particles and wide distributions lead to higher cohesion

Modest changes in particle size / distribution can impact flow.



Low- to high-RPM



Current Knowledge Gap

- Lack of sufficient data on correlations between particle size & distribution, and flowability of granular biomass.

Achievement

- Characterized shear and frictional properties of loblolly pine in a range of particle sizes and **multiple measurement scales.**
- Correlated this bench-top multiscale characterization with pilot-scale flow performance in a wedge hopper and screw conveyor.
- Introduced experiment-informed hypotheses about how size / distributions impact flow rate, consistency, & power consumption.

Industry Impact

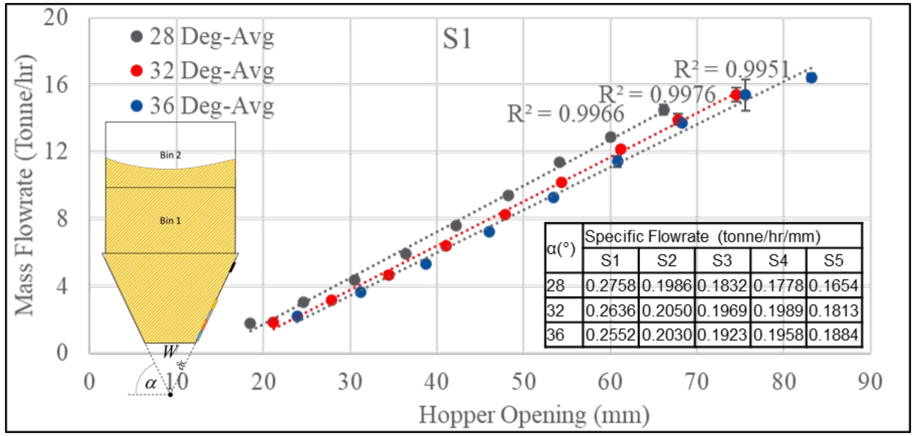
- Industry stakeholders can use these findings as guidance in 0^{th} order diagnostics and equipment design to help identify CMAs and CPPs that need de-risking in their process.

OPEN ACCESS *Work published in "Multiscale Shear Properties and Flow Performance of Milled Woody Biomass", Frontiers in Energy Research (2022) 10.* https://doi.org/10.3389/fenrg.2022.855289

Validation at Pilot-Scale: Hopper Discharge & Screw Conveyor Performance of Milled Pine

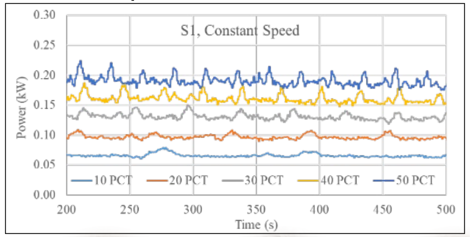
Knowledge

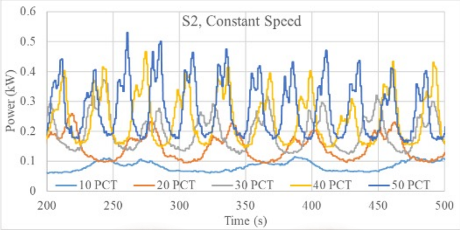
Characterize flow behavior and stability in pilot scale hopper and conveyor.



α(°)	Specific Flowrate (tonne/hr/mm)				
	S1	S2	S3	S4	S5
28	0.2758	0.1986	0.1832	0.1778	0.1654
32	0.2636	0.2050	0.1969	0.1989	0.1813
36	0.2552	0.2030	0.1923	0.1958	0.1884

Screw conveyor: Modest Changes in Size and morphology can have drastic impact on flow forces and stability





Current Knowledge Gap

- Current models for predicting flow performance and hopper geometries are based exclusively on materials testing or on semi-empirical models that breakdown for complex materials.

Achievement

- **Wedge hopper** – identified 1) critical PPs: **hopper scale** & **semi-angle** that influence CQAs (**flow upsets** & **flow rate**); 2) critical MAs: **particle size** & **distribution**, and **moisture**.
- **Screw conveyor** – identified 1) critical PPs: **rotation speed** that influences CQAs (**flow stability** & **power consumption**); 2) critical MAs: **particle size** & **distribution**.

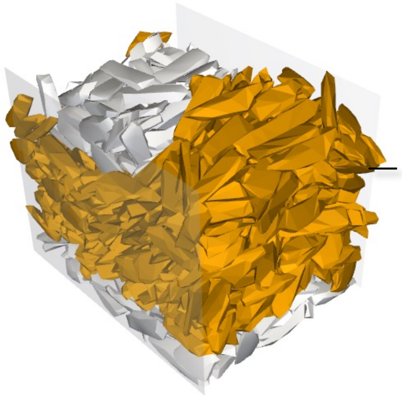
Industry Impact

- Understanding how material properties and equipment design and operation impact flow will elucidate design & robust testing and process equipment for bioenergy feedstocks.

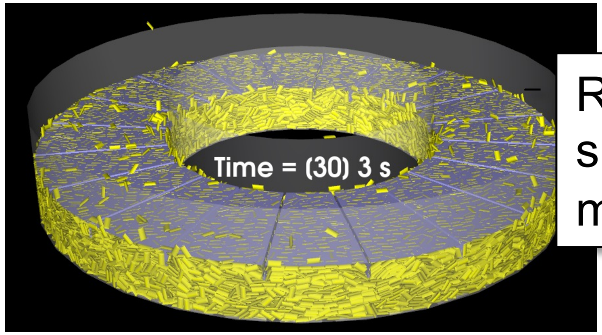
Microscopic to Macroscopic Flow Models for Granular Biomass and MSW

Tools

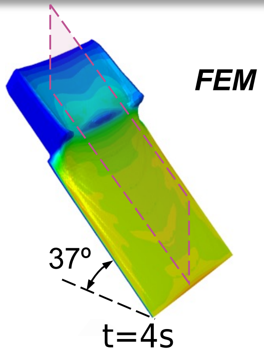
Particle scale | **Pre-pilot scale** | **Pilot scale**



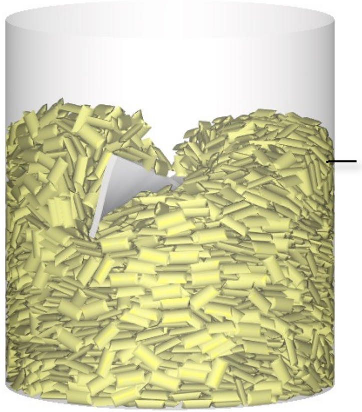
Reciprocating tribometer model



Ring shear model

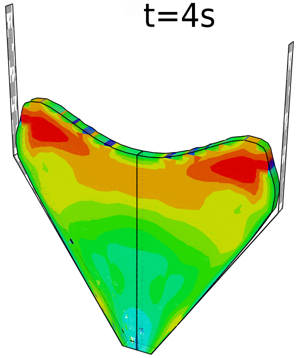


Inclined plane flow model

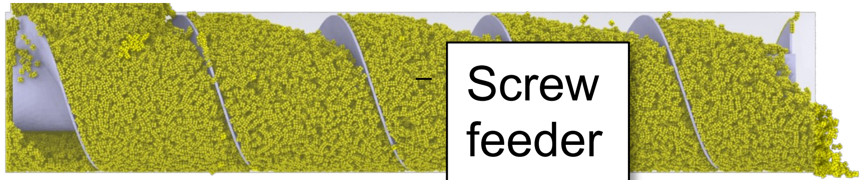


Powder rheometer model

Axial load cell model



Adjustable flow hopper model



Screw feeder model

Particle-resolved Model Elucidates Fundamental Mechanisms of Hopper Clogging

Knowledge

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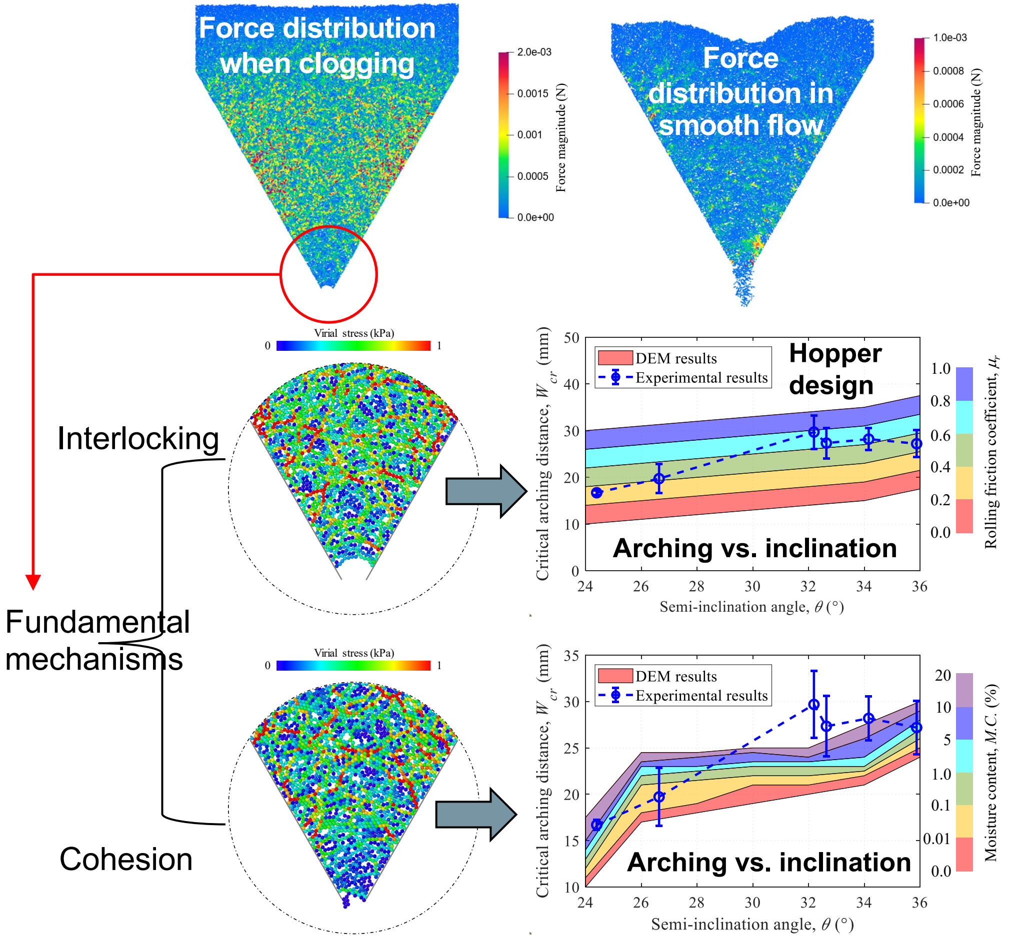
U.S. DEPARTMENT OF ENERGY

Influence of particle interlocking and moisture (cohesion) on hopper flow



Current Knowledge Gap

- Physical experiment alone cannot decouple the influences of particle interlocking and moisture content on flowability.

Achievement

- DEM simulations verified criticality of hopper PPs (opening and inclination angle) from physical experiments
- DEM simulations unveiled two hopper-clogging mechanisms related to particle interlocking and moisture-induced cohesion.
- DEM simulations, upon experiment-informed calibration, provided expanded safe working envelope of hopper flow.

Industry Impact

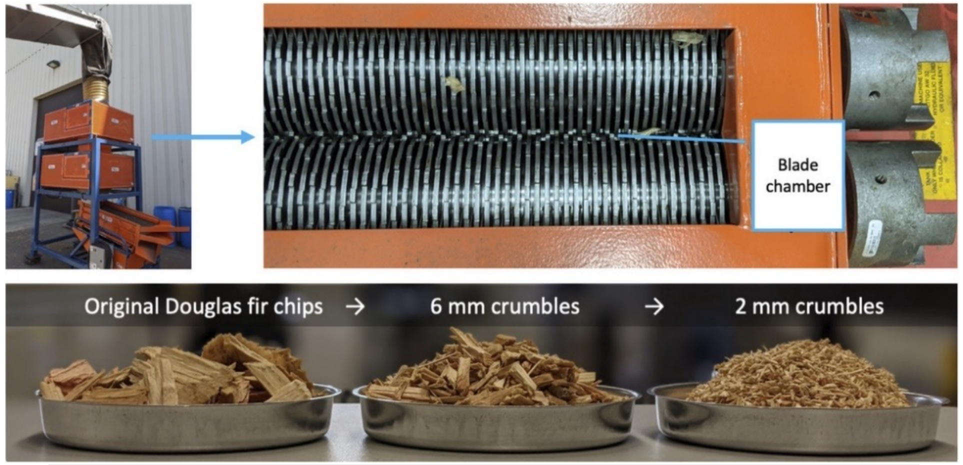
- Industry stakeholders can use this simulation toolkit to assist proof-of-concept design of new material handling equipment for MAs and PPs not easily accessible in limited lab environment.

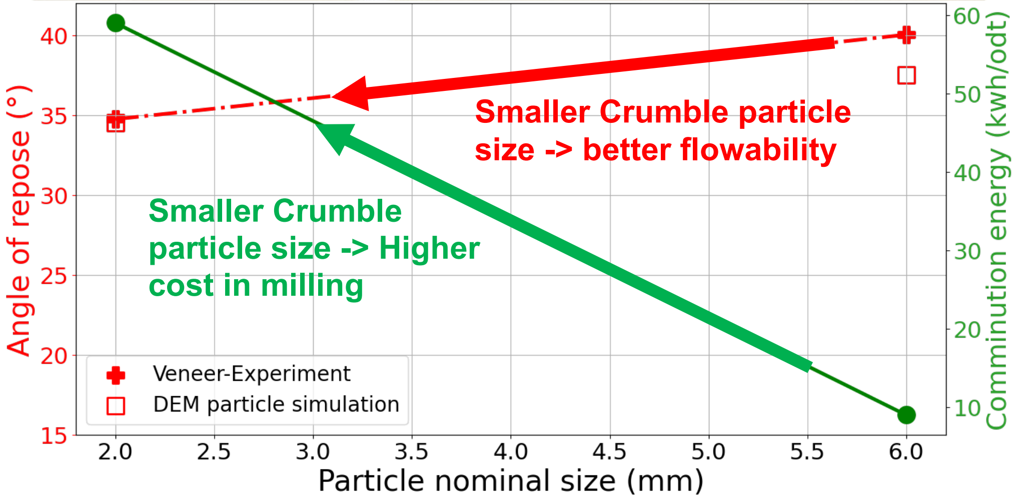
Work published in "Hopper discharge flow dynamics of milled pine and prediction of process upsets using the discrete element method." Powder Technology 415 (2023): 118165. [URL]

Particle-resolved Model Reveals Relations between Milling Energy and Particle Flowability

Knowledge

Influence of particle size & shape on comminution energy and flowability





Current Knowledge Gap

- Lack of sufficient data on relations between particle shape & size, milling energy, and flowability of granular biomass.

Achievement

- Measured angle of repose as flowability metric for FC Crumbler size-reduced Douglas Fir particles at two sizes (2mm vs. 6mm).
- Summarized comminution energy of FC Crumbler to enable TEA.
- DEM simulations identified interparticle locking induced by surface roughness is dominant mechanism in free-surface flow.

Industry Impact

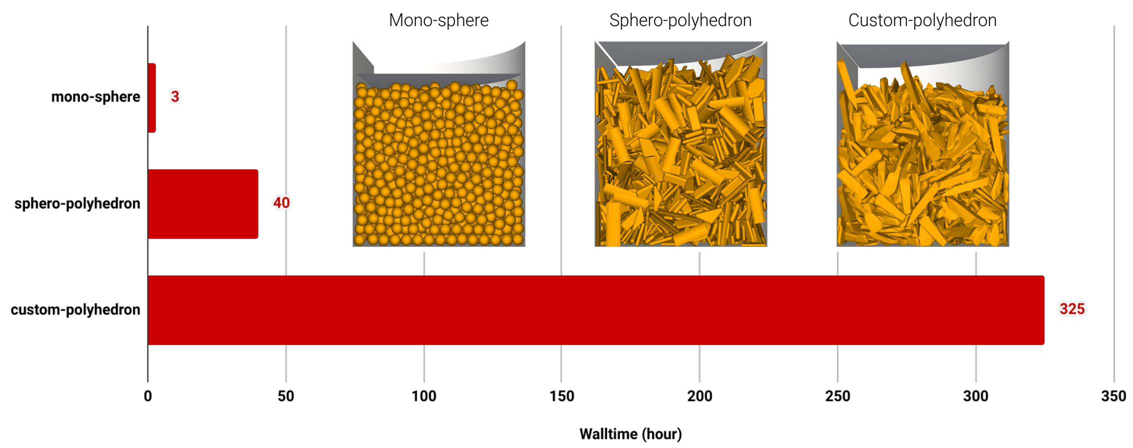
- Industry stakeholders can use the findings as guidance to identify CMAs and jointly optimize the granular biomass flow properties and comminution energy consumption.

OPEN ACCESS

Work published in "Flowability of Crumbler rotary shear size-reduced granular biomass: An experiment-informed modeling study on the angle of repose." Frontiers in Energy Research, section Bioenergy and Biofuels 10 (2022): 859248 [URL]

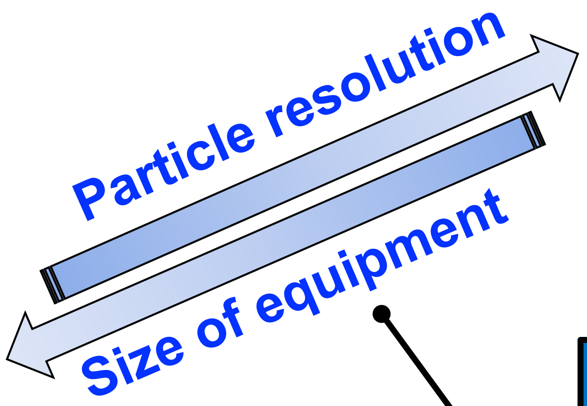
Co-published with industry stakeholder
Co-support from CCPC DFO

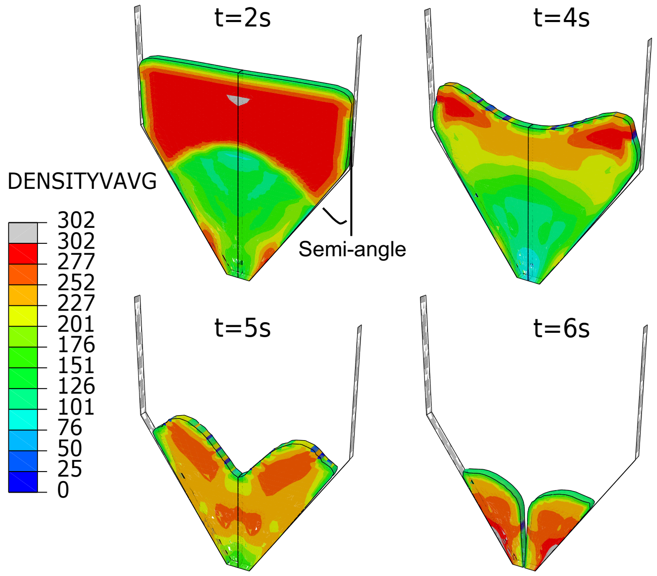
Limitations of Particle-resolved Flow Models



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**

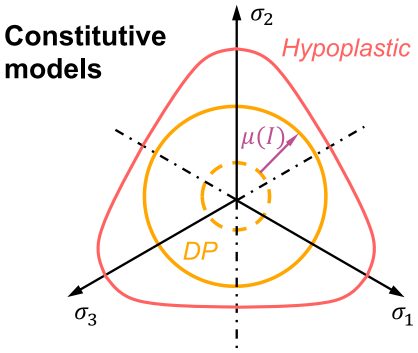
No access to HPC?
Not a problem.

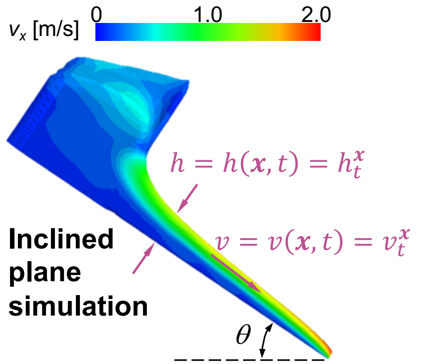
Most simulations shown here require only a good personal workstation to complete within a reasonable amount of time.

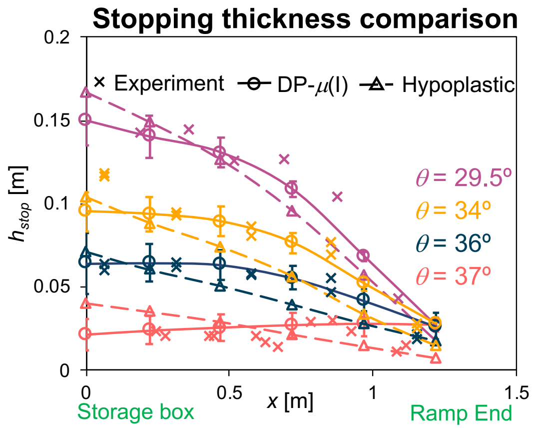
Continuum-mechanics Model Predicts Quasi-static to Dense Flow Regime Transition At-Scale

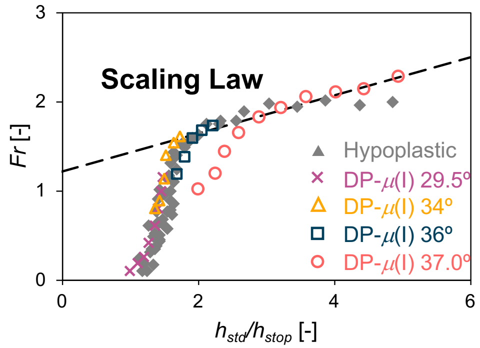
Knowledge

Investigated granular biomass flow regime transition using experiments and simulations of inclined plane flow









Current Knowledge Gap

- Conventional granular flow in quasi-static regime (constant internal friction angle) at low flow rate and transit in dense regime (friction angle is a function of flow rate) at high flow rate.
- Lack of in-situ dependency of internal friction on flow rate.

Achievement

- Developed a new model to allow dynamic internal friction angle; In contrast, traditional Computational Fluid Dynamics (CFD)-derived models assuming fluid-like properties (scalar pressure) for biomass proven to not work.
- Validated the the new DP-u(I) model against lab flowability tests and inclined plane flow tests.
- The new DP-u(I) model is more accurate for high-speed flow.

Industry Impact

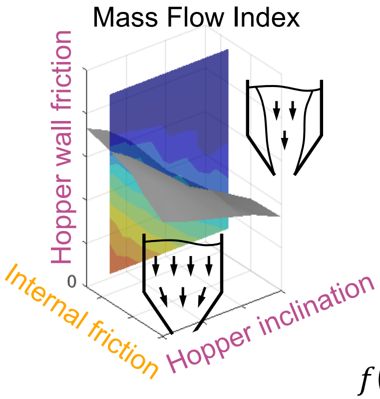
- For handling operations with a high flow rate, the new model is essential to accurately predict the flow behavior and throughput.

Manuscript entitled “Characterization and modeling on the multi-regime flow behavior of particulate biomass”, In preparation

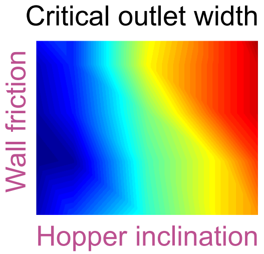
Wedge Hopper Design for Woody Biomass

Created wedge hopper design chart for woody biomass to avoid funnel flow and hopper arching and to predict throughput

Mass Vs. Funnel flow



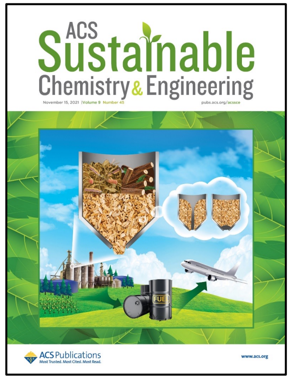
Hopper arching



Flow throughput

$$f(\rho_p, d_{50}, \phi_c, L, W, \mu) = \text{Mass flow rate}$$

Material attributes **Hopper parameters**



On journal cover page – "Flow and arching of biomass particles in wedge-shaped hoppers." ACS Sustainable Chemistry & Engineering 9.45 (2021): 15303-15314. [URL]

"Wedge-Shaped Hopper Design for Milled Woody Biomass Flow", ACS Sustainable Chemistry & Engineering 10, 50 (2022): 16803-16813 [URL].

Description

- Validated flow models confirm 3 CMAs (hopper inclination, wall friction, and material internal friction) that dictate flow patten for dry woody biomass feedstock. Parameter space of the 3 CMAs defined to distinguish mass flow and funnel flow.
- A critical arching distance design chart is created in the space of two CPPs (wall friction and hopper inclination)
- Developed a predictive equation for flow throughput under mass flow regime with particle density, average particle size, internal friction, hopper outlet width & length, and inclination as inputs.

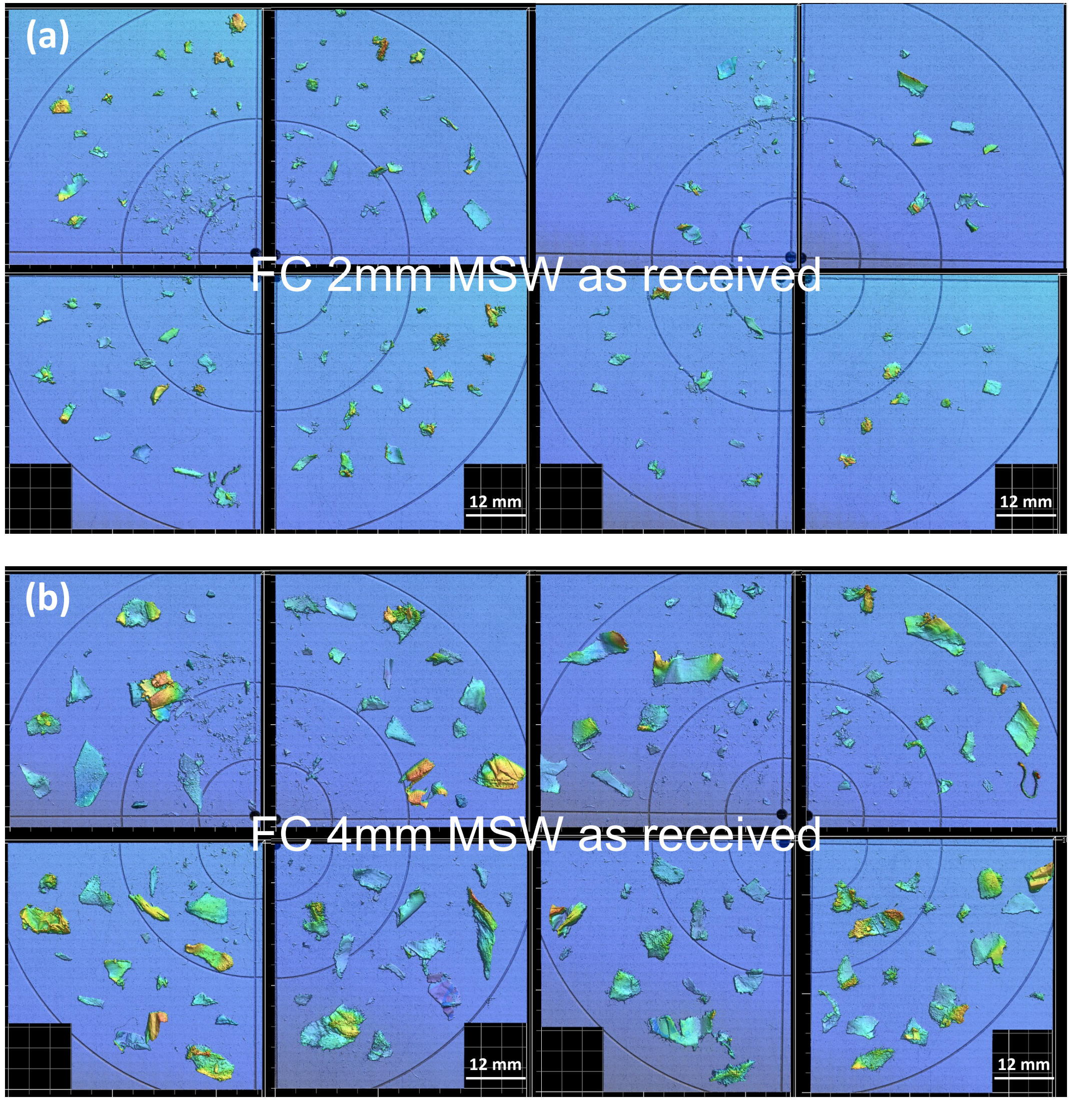
Value of new tool

- First-of-its-kind design charts for dry woody biomass hopper flow.
- The design charts can be used to quickly assess wedge-shaped hopper design to avoid funnel flow and hopper arching.

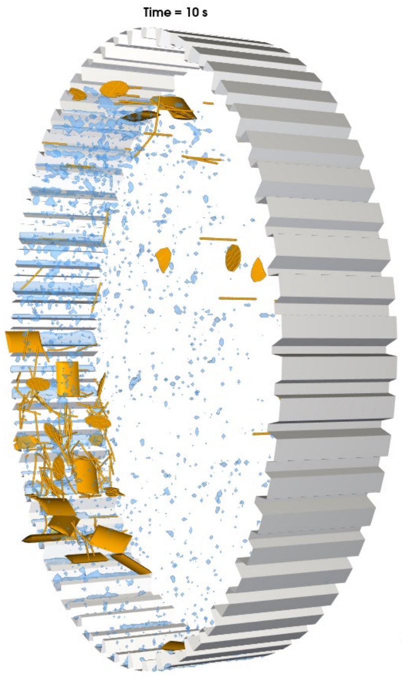
Industry Impact

- Both the flow simulation tool and design charts are products of FCIC to assist the bioenergy industry for handling unit design.

Ongoing: True Particle Shape & Size Measurement for Milled MSW and Flow Modeling

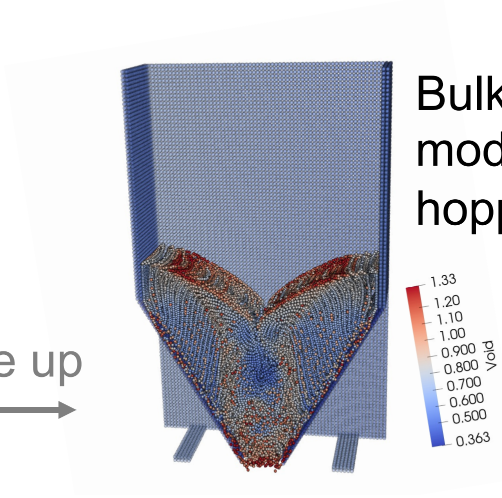


Pathway to flow modeling for milled MSW by developing resolved-particle flow model and CFD-type bulk-scale flow model for design guide

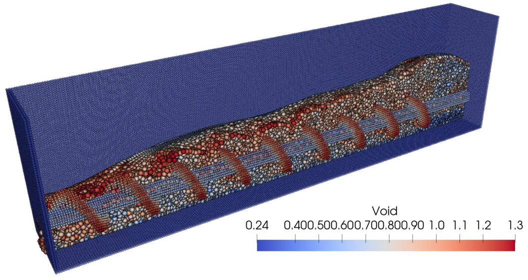


Resolved-particle model

Scale up



Bulk flow model for hopper



Bulk flow model for auger

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)

3 – Impact Public Release of Open-Source Granular Flow Simulation Toolkits

Tools

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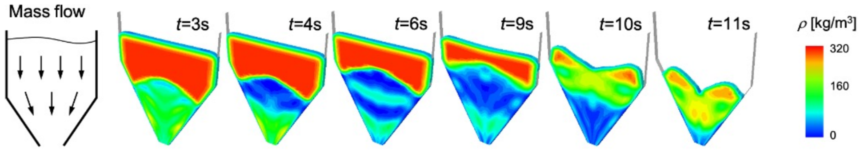
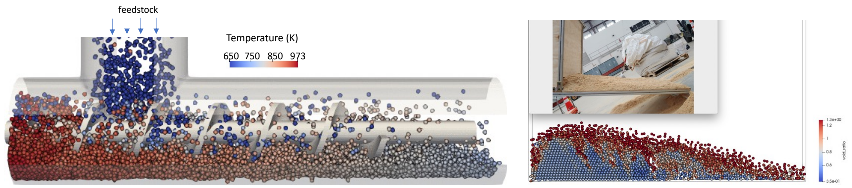
Three open-source granular material-flow simulation software packages.

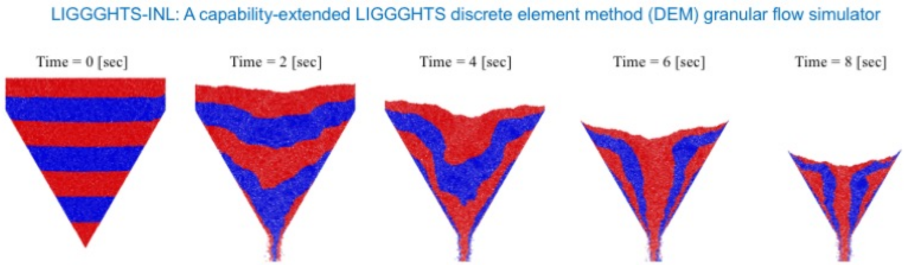
Software #1: Granular Flow Models (by INL)



Software #2: BDEM and Exagoop (by NREL)



Software #3: LIGGGHTS-INL (by INL)



Description

- GranularFlowModels [URL]: continuum flow model in Abaqus / Explicit User MATerial subroutine (VUMAT) add-on modules.
- BDEM/ Exagoop [URL]: GPU accelerated discrete and material-point method solvers using exascale computing tools.
- LIGGGHTS-INL [URL]: a capability-extended LIGGGHTS discrete element method particle simulation software.

Value of new tool

- For creating **hopper design charts**, based on and expanded from experimental data of multiscale flow characterization.

Industry Impact

- Applications for GTI, Forest Concepts, BHS, AdvanceBio, etc.

GTI ENERGY · forestconcepts™ bioenergy · BHS BulkHandling SYSTEMS · advancebio Fuel & Chemical Technologies

Software #1 publications: 1) Powder Technology 368 (2020): 45-58. 2) Powder Technology 383 (2021): 396-409. 3) ACS Sustainable Chemistry & Engineering 9, 45 (2021): 15303-15314. 4) Frontiers in Energy Research, section Bioenergy and Biofuel (2022): 855848. 5) ACS Sustainable Chemistry & Engineering 10, 50 (2022): 16803-16813.
Software #3 publications: 1) Powder Technology 345 (2019): 1-14. 2) Biomass & Bioenergy 141 (2020): 105649. 3) Powder Technology 385 (2021): 557-571. 4) Powder Technology 397 (2022): 117100. 5) Frontiers in Energy Research, section Bioenergy and Biofuel (2022): 859248. 6) Frontiers in Energy Research, section Bioenergy and Biofuel (2022): 855848. 7) Powder Technology 409 (2022): 117797. 8) Powder Technology 415 (2023): 118165.

Summary

Objective:

Develop first principles-based design tools that enable continuous, steady, trouble-free bulk flow transport through processing train to reactor throat and enable applications of the developed tools to industry stakeholders.

Technical Approach:

This task has established an integrated multiscale experimental and physics-based modeling approach.

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.

Achievements:

- Fundamental knowledge of biomass flow physics from lab scale to pilot scale.
- Multiscale biomass flow characterization test approaches and handling equipment design charts.
- Open-source computational granular flow simulation toolkits.
- High-impact-factor journal articles & conference; expanded collaborations with industry stakeholders.

Quad Chart Overview

Timeline
- *October 1, 2021*
- *September 30, 2024*

	FY22 Costed	Total Award
DOE Funding	$1,710,000	
Project Cost Share *	NA	NA

TRL at Project Start:

TRL at Project End:

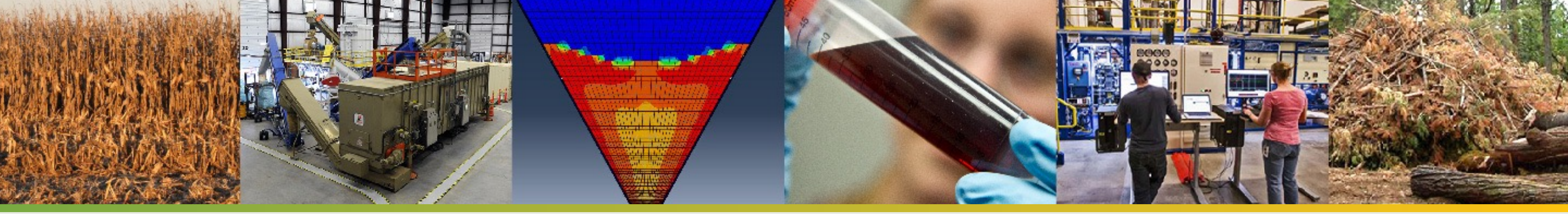
Project Goal
Complete reliable working envelopes of CMAs and CPPs for CQAs of operation units, e.g., design charts for consistent flow; dissemination of validated design tools (design charts, open-source flow simulation codes) for equipment designers.

End of Project Milestone
(INL): Hopper design chart for milled corn & controlled blends of corn-wastepaper in 5%-20% M.C. Flow simulations achieve >80% agreement with physical tests on discharge flow rate and critical arching distance of hopper for controlled corn-wastepaper blends in low to mid moisture content.

Funding Mechanism
2021 Lab Call – FCIC Merit Review

Project Partners*
- Partner 1
- Partner 2

*Only fill out if applicable.



Additional Slides

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Responses to Previous Reviewers' Comments

- "Can these tools be demonstrated with real world utilization? Can the team solve a known problem with these tools and apply TEA to demonstrate the benefit?" **Reply:** One of the largest and most direct benefits to the economics of a process is through avoidance of process upsets and downtime. The tools we have been continuously developing are being demonstrated in practical hopper discharge and screw conveyer operations. Specifically, the development and validation testing for this task take place at INL in a custom angle-adjustable hopper, on the scale of 5-15 tons/hr. and demonstrated the operating conditions needed to avoid process upsets like hopper arching. While production-scale operations are certainly at higher capacities, this work demonstrated a clear step forward.

- "The hopper flow model should be validated at larger scale." **Reply:** Pilot-scale (5-15 tons/hr.) and even production-scale (30-80 tons/hr.) hopper flow is within the sight of our project. To overcome the high cost of obtaining experimental hopper flow data in these scales, FCIC has been seeking a viable pathway to forge industrial collaboration through BETO Direct Funding Opportunities (DFO).

- "It's not clear if the models are "user friendly" enough for non-experts to utilize to investigate the impact of their specific MA's on equipment design and operation." **Reply:** We agree that the current version of the models will not be very "user friendly". In the engineering software industry, a user-friendly simulation package is normally the result of decade-long iterative effort in core feature and user-interface development & enhancement. User feedback is critically important to allow developers to plan how to continuously improve the user experience. Our open-source software strategy allows us to release the package and provide detailed user manual and examples for "non-experts".

Publications and Presentations

Journal articles (FY22 – present)

- F. Chen, Y. Xia, J. Klinger, Q. Chen, "Hopper discharge flow dynamics of milled pine and prediction of process upsets using the discrete element method." Powder Technology 415 (2023): 118165. https://doi.org/10.1016/j.powtec.2022.118165
- N. Saha, C. Goates, S. Hernandez, W. Jin, T. Westover, J. Klinger. "Characterization of particle size and moisture content effects on mechanical and feeding behavior of milled corn (Zea mays L.) stover." Powder Technology (2022), 117535. https://doi.org/10.1016/j.powtec.2022.117535
- J. Klinger, N. Saha, T. Bhattacharjee, S. Carilli, W. Jin, Y. Xia, R. Daniel, C. Burns, O. Ajayi, Z. Cheng, R. Navar, T.A. Semelsberger, "Multiscale Shear Properties and Flow Performance of Biomass." *Frontiers in Energy Research / Bioenergy and Biofuels* (2022). https://doi.org/10.3389/fenrg.2022.855289
- W. Jin, Y. Lu, F. Chen, A. Hamed, Y. Xia, N. Saha, J. Klinger, S. Dai and Q. Chen, "On the fidelity of computational models for the flow of milled loblolly pine: A benchmark study on continuum-mechanics models and discrete-particle models." *Frontiers in Energy Research Bioenergy and Biofuels* (2022). Accepted.
- A. Hamed, Y. Xia, N. Saha, J. Klinger, D. N. Lanning, J. Dooley, "Flowability of Crumbler rotary shear size-reduced granular biomass: An experiment-informed modeling study on the angle of repose." *Frontiers in Energy Research / Bioenergy and Biofuels* 10 (2022). https://doi.org/10.3389/fenrg.2022.859248
- Y. Lu, W. Jin, J. Klinger, S. Dai. "Flow and Arching of Biomass Particles in Wedge-Shaped Hoppers." *ACS Sustainable Chemistry & Engineering* 9, No. 45 (2021): 15303-15314. https://doi.org/10.1021/acssuschemeng.1c05628
- F. Chen, Y. Xia, J. Klinger, Qiushi Chen, "A set of hysteretic nonlinear contact models for DEM: Theory, formulation, and application for lignocellulosic biomass." *Powder Technology* 397 (2022): 117100. https://doi.org/10.1016/j.powtec.2021.117100
- Z. Cheng, D.W. Gao, F.M. Powers, R. Navar, J.H. Leal, O.O. Ajayi, T.A. Semelsberger, "Effect of Moisture and Feedstock Variability on the Rheological Behavior of Corn Stover Particles." *Frontiers in Energy Research* 10 (2022): 868050. https://doi.org/10.3389/fenrg.2022.868050
- J.H. Leal, E.J. Meierdierks, R. Navar, C.M. Moore, A.E. Ray, T.A. Semelsberger, "Impacts of biologically induced degradation on surface energy, wettability & cohesion of corn stover." *Frontiers in Energy Research / Bioenergy and Biofuels* (2022). https://doi.org/10.3389/fenrg.2022.868019
- R. Navar, J.H. Leal, B.L. Davis, T.A. Semelsberger, "Rheological effects of Moisture Content on the Anatomical Fractions of Loblolly Pine (*Pinus taeda*)", *Powder Technology* (2022). 412, 118031. https://doi.org/10.1016/j.powtec.2022.118031

Publications and Presentations (continued)

Conference presentations/proceedings (FY22 – present)

- W. Jin, Y. Lu, J. Klinger, Y. Xia. "Continuum-Mechanics-Based Flow Modeling of Particulate Milled Biomass." Presented at 2022 AIChE Annual Meeting, Phoenix, Arizona, November 13-18, 2022.
- Y. Xia, W. Jin, A. Hamed, J. Klinger, N. Saha, T. Bhattacharjee, V. Thompson, C. L. Williams, D. Thompson, L. Wendt. "Multiphysics-Resolved Digital Twins of Feedstock Preprocessing and Handling Unit Operations: Recent Progress and Best Practices." Presented at 2022 AIChE Annual Meeting, Phoenix, Arizona, November 13-18, 2022.
- F. Chen, Y. Xia, Q. Chen. "Discrete Element Modeling of Wedge Hopper Discharge of Loblolly Pine Chips." Presented at 2022 AIChE Annual Meeting, Phoenix, Arizona, November 13-18, 2022.
- J. Klinger, T. Bhattacharjee, N. Saha, S. Carilli, N. Berglund, W. Jin, Y. Xia. "Mechanical and Flow Characterization of Loblolly Pine Residues." Presented at 2022 AIChE Annual Meeting, Phoenix, Arizona, November 13-18, 2022.
- A. Hamed, Y. Xia, N. Saha, J. Klinger, D. Lanning and J. Dooley. "Investigation of Particle Characteristics Influence of Crumbler® Rotary Shear Comminuted Granular Biomass on the Performance of Screw Feeding: Modeling and Experiment." Presented at 2022 AIChE Annual Meeting, Phoenix, Arizona, November 13-18, 2022.
- A. Hamed, Y. Xia, J. Klinger, D. N. Lanning, J. Dooley. "Flowability of Crumbler® rotary shear size-reduced granular biomass: An experiment-informed", Presented at 2022 ASABE Annual International Meeting, Houston, Texas, July 17-20, 2022.
- Q. Chen, F. Chen, Y. Xia. "Discrete Element Modeling of Wedge Hopper Discharge of Milled Loblolly Pine", Presented at 2022 ASABE Annual International Meeting, Houston, Texas, July 17-20, 2022.
- Y. Xia, F. Chen, J. Klinger, and Q. Chen. "A Class of Generalized Strain-Hardening Discrete Element Method (DEM): Theory, LIGGGHTS Open-Source Implementation, and Applications for Granular Biomass Flow." Presented at 2021 AIChE Annual Meeting (Virtual), November 7-19, 2021.
- Y. Xia, F. Chen, J. Klinger, J. Kane, T. Bhattacharjee, R. Seifert, O. Ajayi, and Q. Chen."A Nano-CT Informed Polyhedral Discrete Element Modeling Approach for Flow of Complex-Shaped Granular Woody Biomass." Presented at 2021 AIChE Annual Meeting (Virtual), November 7-19, 2021.
- Y. Xia, W. Jin, J. Klinger, T. Bhattacharjee and V. Thompson. "Recent Progress on the Development of a Virtual Feedstock Preprocessing & Handling Laboratory". Presented at 2021 AIChE Annual Meeting (Virtual), November 7-19, 2021.

Open-source flow simulation package repositories

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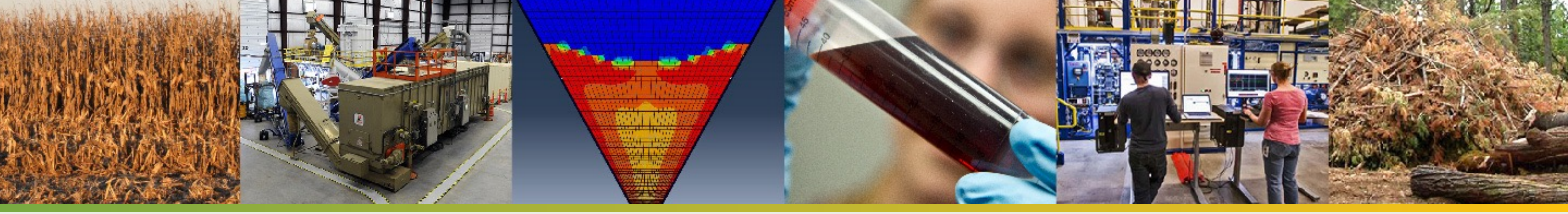
- GranularFlowModels: continuum flow model in Abaqus / Explicit User MATerial subroutine (VUMAT) add-on modules.
  - https://github.com/idaholab/GranularFlowModels
- LIGGGHTS-INL: a capability-extended LIGGGHTS discrete element method particle simulation software.
  - https://github.com/idaholab/LIGGGHTS-INL
- BDEM/ Exagoop: GPU accelerated discrete and material-point method solvers using exascale computing tools.
  - https://github.com/idaholab/GranularFlowModels



Additional Project Achievements

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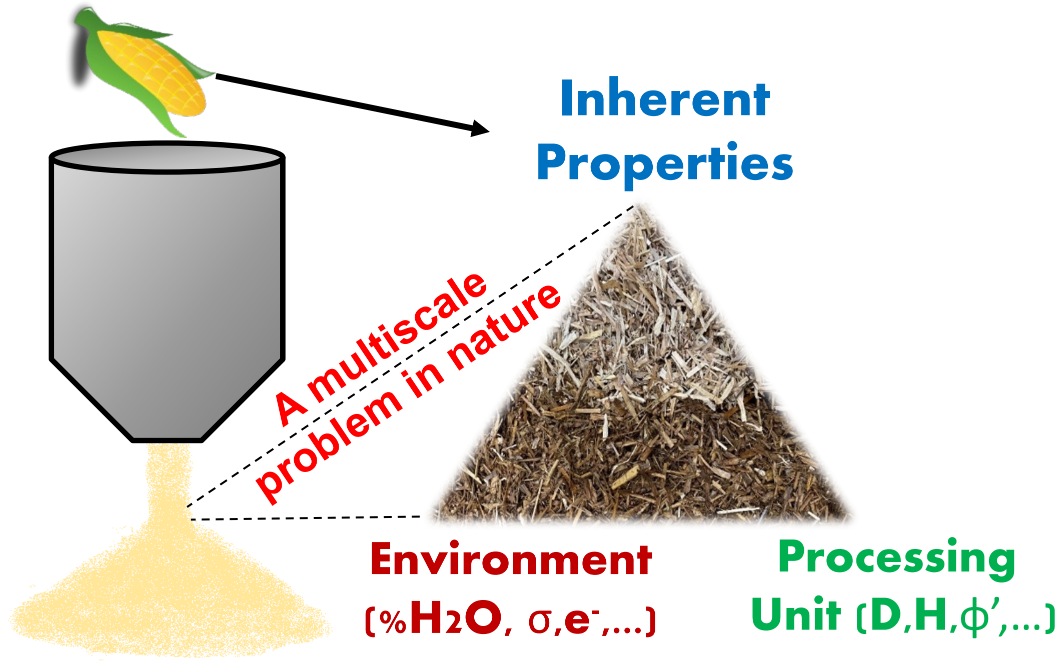
Question: How and What to Measure about Flow Behavior of Granular Biomass

Knowledge

It's imperative to test each powder because the flow behavior of a powder is determined by its inherent properties, the environment, and the processing unit it's in.



Work published in "Flow Behavior Characterization of Biomass Feedstocks", Powder Technology (2021) 387, 156-180, DOI: 10.1016/j.powtec.2021.04.004

Current Knowledge Gap

- Existing powder processing/handling equipment are mostly designed for coal and pharmaceutical ingredients
- Biomass encounters flow stoppages in these repurposed equipment, hampering process economics
- Lack of knowledge on the unique flow behavior of biomass

Achievement

- **Discussed** how powder flow behavior depends on the inherent properties, environment, and processing equipment
- **Reviewed** literature on the characterization of biomass powder flow behavior using shear tester & powder rheometer
- **Proposed** complementing powder rheometry with surface energy measurements, tribometry and DEM modeling to elucidate the flow behavior of granular biomass

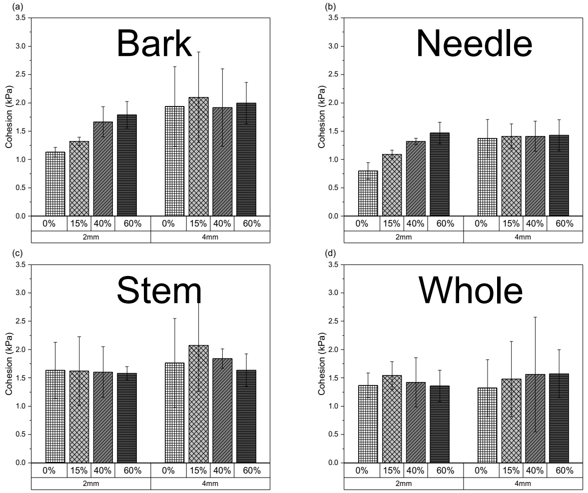
Industry Impact

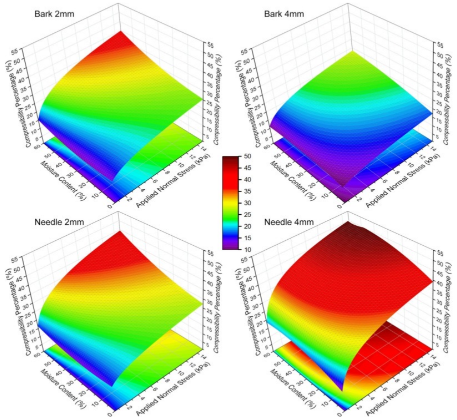
- Co-reviewed and -published with **industry stakeholder** to ensure FCIC Material Handling Task research direction is aligned with industry driven grand challenges

Lab-Scale Flow Characterization of Loblolly Pine Anatomical Fractions

Knowledge

Moisture content and its influence on loblolly pine anatomical fractions





Work published in "Rheological effects of Moisture Content on the Anatomical Fractions of Loblolly Pine (Pinus taeda)", Powder Technology (2022). 412, 118031
https://doi.org/10.1016/j.powtec.2022.118031

Current Knowledge Gap

- Minimal information related to the flowability of loblolly pine: 1) influence of moisture content; 2) Little to no studies of the rheological properties of loblolly pines' anatomical fractions.

Achievement

- Assessed the moisture contents' effect on 3 anatomical fractions and 1 mixture at 2 particle sizes. Flowability of stem particles doesn't change with moisture → more predictable handling.
- Smaller particle size resulted in less change in cohesive strength, shear stress, compressibility) and thus more consistent handling.

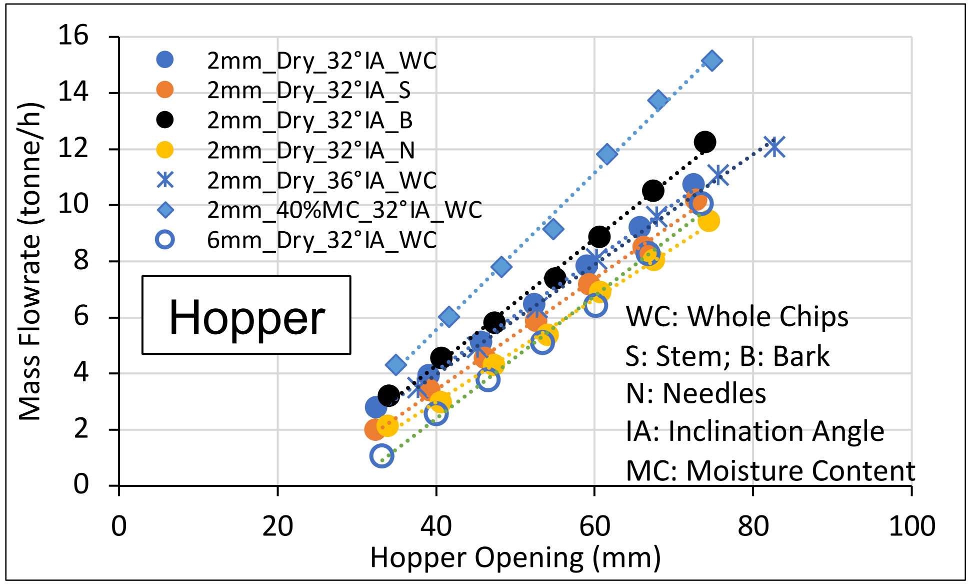
Industry Impact

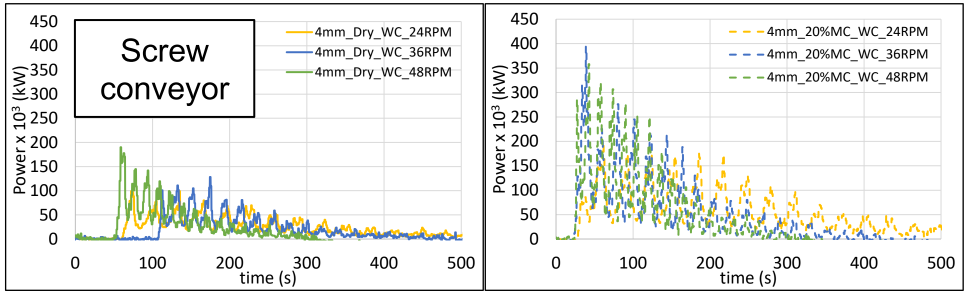
- Comprehensive evaluation of how anatomical fractions behave under moisture can benefit hopper design, consideration the worst-case scenario material and avoiding it.
- Though some fractions exhibit large rheological change with moisture, complex mixtures muted this change, indicating advantages for industry

Pilot-Scale Hopper Flow Characterization of Loblolly Pine Anatomical Fractions

Knowledge

Effect of moisture, particle size, and anatomical fraction of loblolly pine on flowability and power consumption





Current Knowledge Gap

- Minimum data about the flowability of various anatomical fraction of loblolly pine and effect of particle size along with moisture.

Achievement

- **Hopper**: with a fixed hopper opening, increasing particle size leads to the decrease in mass flow rate decreases, while the inclination angle showed minimal effect on mass flow rate.
- **Hopper**: increasing moisture leads to increase in mass flow rate.
- **Hopper**: different anatomic fractions showed different flow patterns; needles (high aspect ratio) showed the worst flowability.
- **Screw conveyor**: Increasing moisture and rotation speed leads to more sporadic power consumptions in magnitude & frequency.

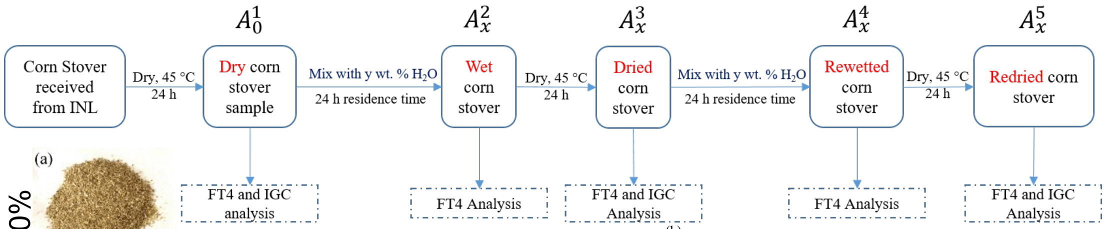
Industry Impact

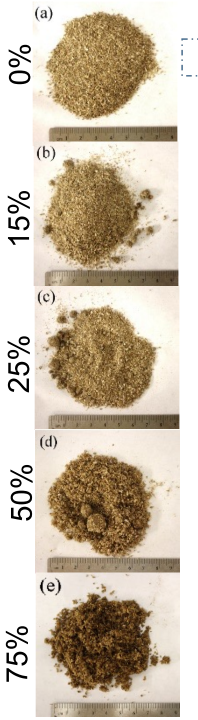
- This study provided extensive data of CMAs, CPPs, CQAs to benefit bioenergy industry’s design hopper and screw feeder.

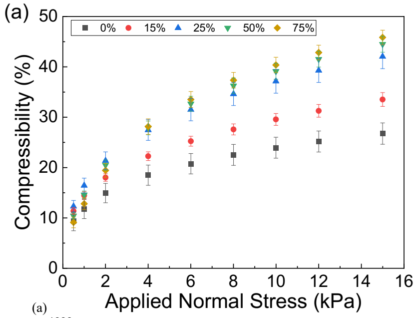
Lab-Scale Flow Characterization of Corn Stover Anatomical Fractions

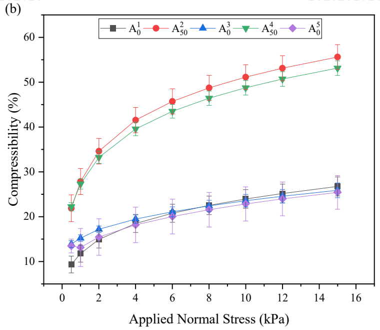
Knowledge

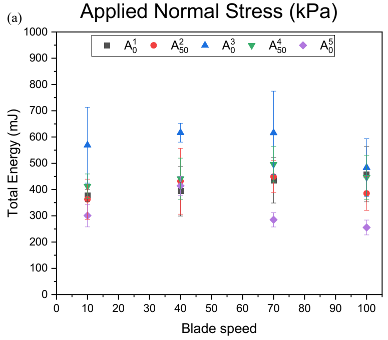
Influence of moisture and continuous drying/wetting of corn stover particles

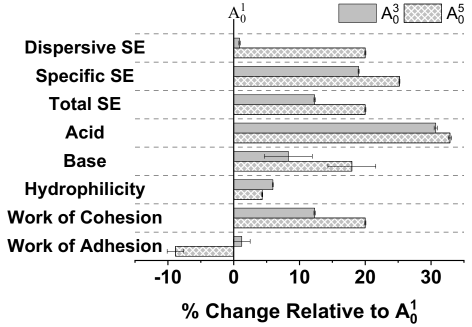












OPEN ACCESS ***"Effect of Moisture and Feedstock Variability on the Rheological Behavior of Corn Stover Particles", Front. Energy Res. (2022). 10, 868050*** https://doi.org/10.3389/fenrg.2022.868050

Current Knowledge Gap

- No studies related to repeated drying and wetting steps of any biomass feedstocks.

Achievement

- Exhibited small differences upon repeatedly drying and wetting the corn stover on the macro scale, primarily on the cohesive strength, indicative of a more free-flowing material.
- Showed increased SE (total - specific, Acid-base) after the 1st wetting/drying step. This continued to increase upon carrying out a 2nd step, with a decrease in its work of adhesion.

Industry Impact

- Most biomass feedstock in storage is in contact with moisture (rainfall, ambient, etc.). A **naturally-occurring drying-wetting procedure** can change the rheological behavior of the biomass.
- Such changes can be crucial for feedstock handling, potentially showing that wetting-drying steps can be a pre-treatment to attain improved flowability, aiding in handling operations.

Pilot-scale Flow of Milled Corn Stover and Relations to Particle Size & Distribution

Knowledge

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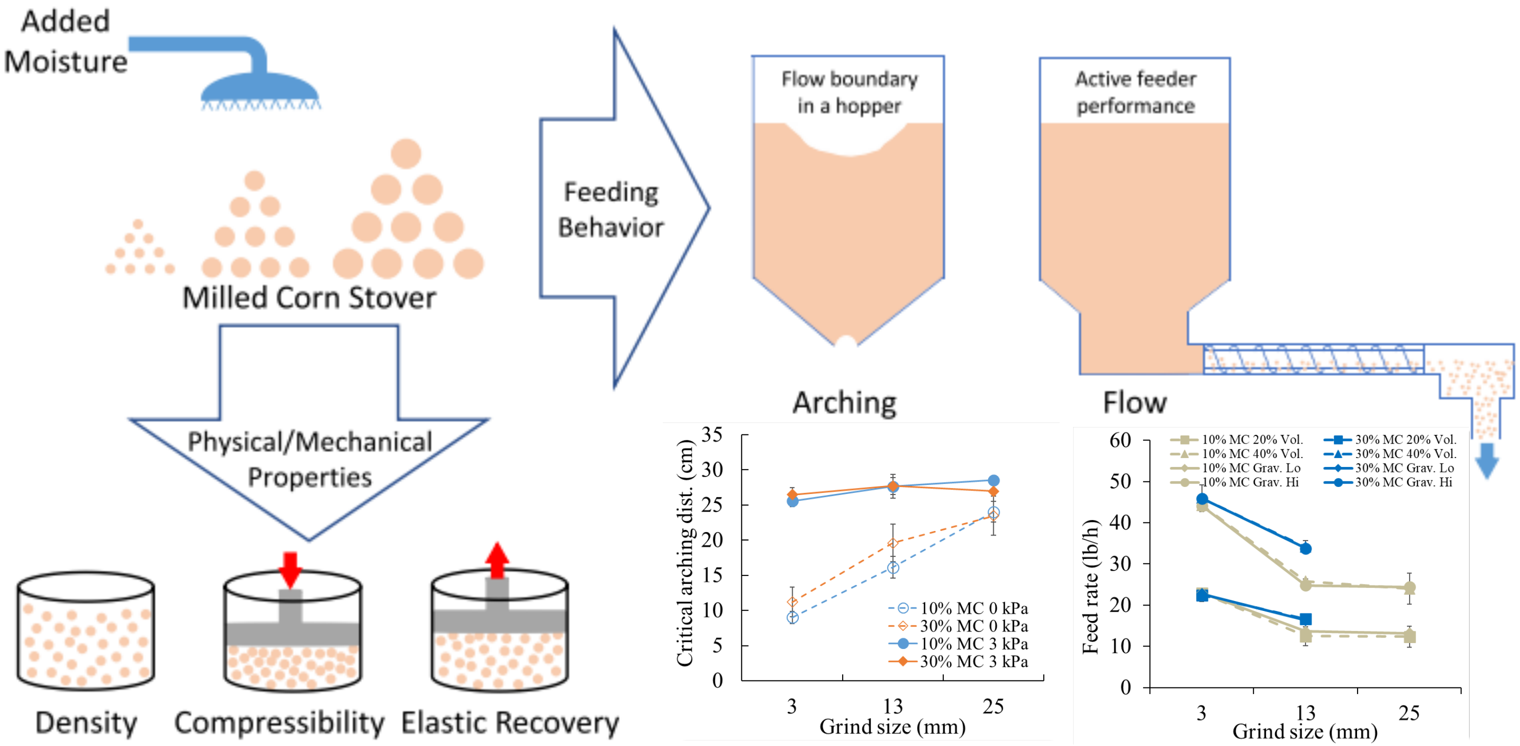
Influence of particle size & distribution on hopper and feeder performance



Work published in "Characterization of particle size and moisture content effects on mechanical and feeding behavior of milled corn (Zea mays L.) stover". Powder Technology (2022): 117535. https://doi.org/10.1016/j.powtec.2022.117535

Current Knowledge Gap

- Lack of sufficient data on relations between CMAs (particle size & distribution) and CQAs flowability of granular biomass.

Achievement

- **Hopper**: arching distance (at low stress) and compressibility increased with corn stover size, while elastic recovery and flow rate decreased.
- **Screw conveyor**: smaller particles flows better (less variability & power consumption); moisture had little impact.

Industry Impact

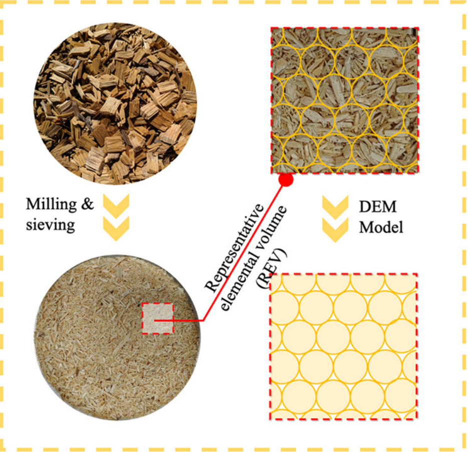
- Industry stakeholders can use these findings as guidance in 0th order diagnostics and equipment design to help identify CMAs and CPPs that need de-risking in their process.

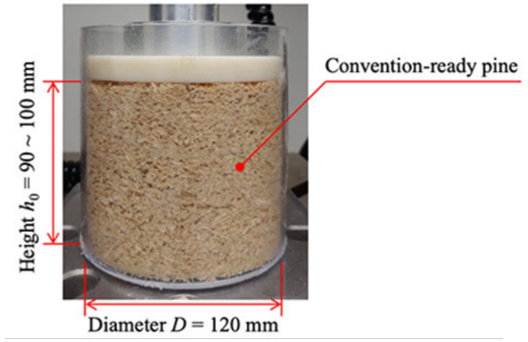
Fundamental Intergranular Contact Physics of Milled Woody Biomass

Tools

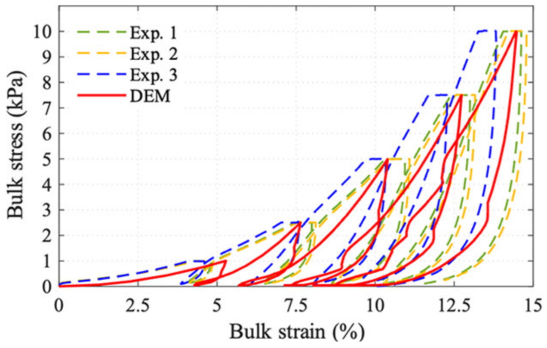
Developed contact physics-resolved DEM models for granular biomass flow

Lignocellulosic biomass & Representative Elementary Volume (REV)





Model development & experimental validation with axial loading tester →



Work published in "A set of hysteretic nonlinear contact models for DEM: Theory, formulation, and application for lignocellulosic biomass." Powder Technology 397 (2022): 117100. https://doi.org/10.1016/j.powtec.2021.117100

Description

- A DEM particle contact model that resolves realistic granular contact behavior of milled pine is developed and implemented in open-source DEM particle simulation software LIGGGHTS-INL.

Value of new tool

- Open-source model maximizes community contribution.
- Adaptable and transferrable as design tool for industries.

Industry Impact

- Feedstock handling equipment suppliers, biorefinery designers.
- For academia as educational tool for DEI & workforce pipeline.

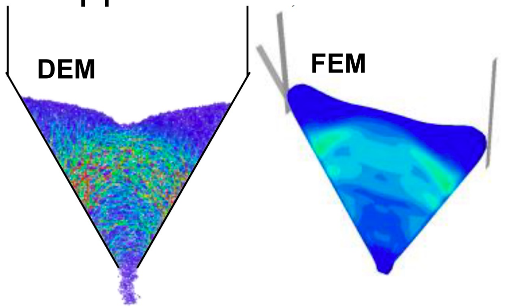
→ Growing user & industry application base

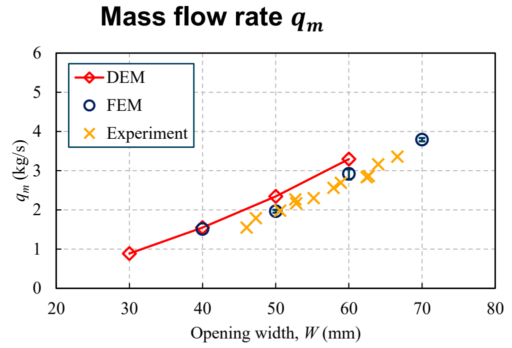
Computational Benchmarks on Granular Flow

Knowledge

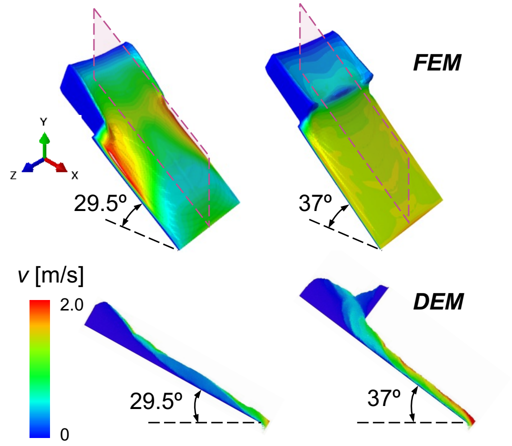
Benchmark the fidelity of continuum-mechanics models and discrete-particle models for flow modeling of milled pine

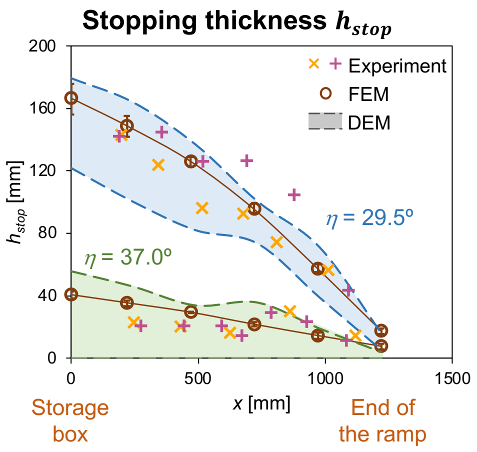
Hopper flow





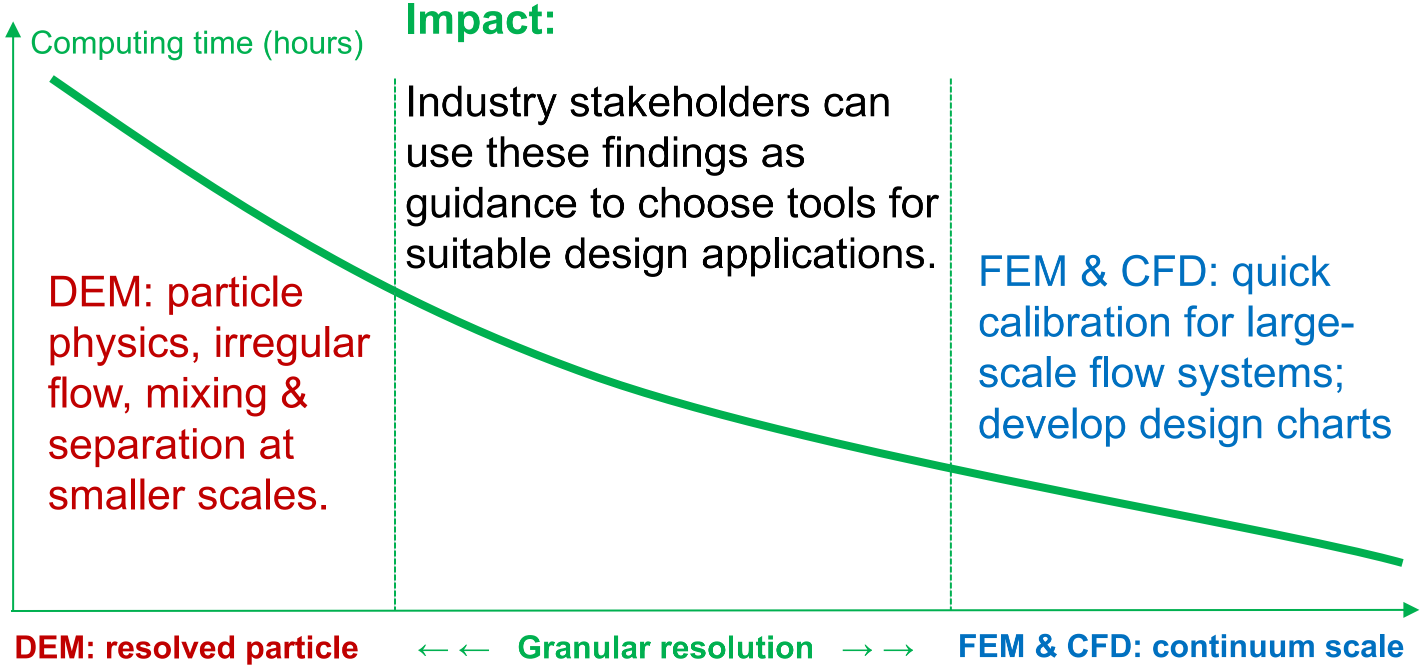
Inclined plane flow





Current Knowledge Gap

- No comparison exists in the flow modeling of granular biomass between continuum-mechanics and discrete-particle models.



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