DOE Bioenergy Technologies Office (BETO)
2019 Project Peer Review

Integrated Process Optimization for Biochemical Conversion

March 7, 2019

Advanced Development and Optimization: Analysis and Modeling

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Goal Statement

The **goal** is to ***reduce the cost of producing biofuels by designing a reliable, cost effective, sustainable, robust system for feeding of biomass feedstocks to the reactor*****.**

Outcomes

1. An optimized feeding system design – from biomass grinding to the reactor throat – which ensures reactor reliability nearly 90% for biomass with 10-30% moisture and 5-15% ash contents.
2. A demonstration of the proposed design at 1DMT/day for 2 weeks at INL's process demonstration unit.

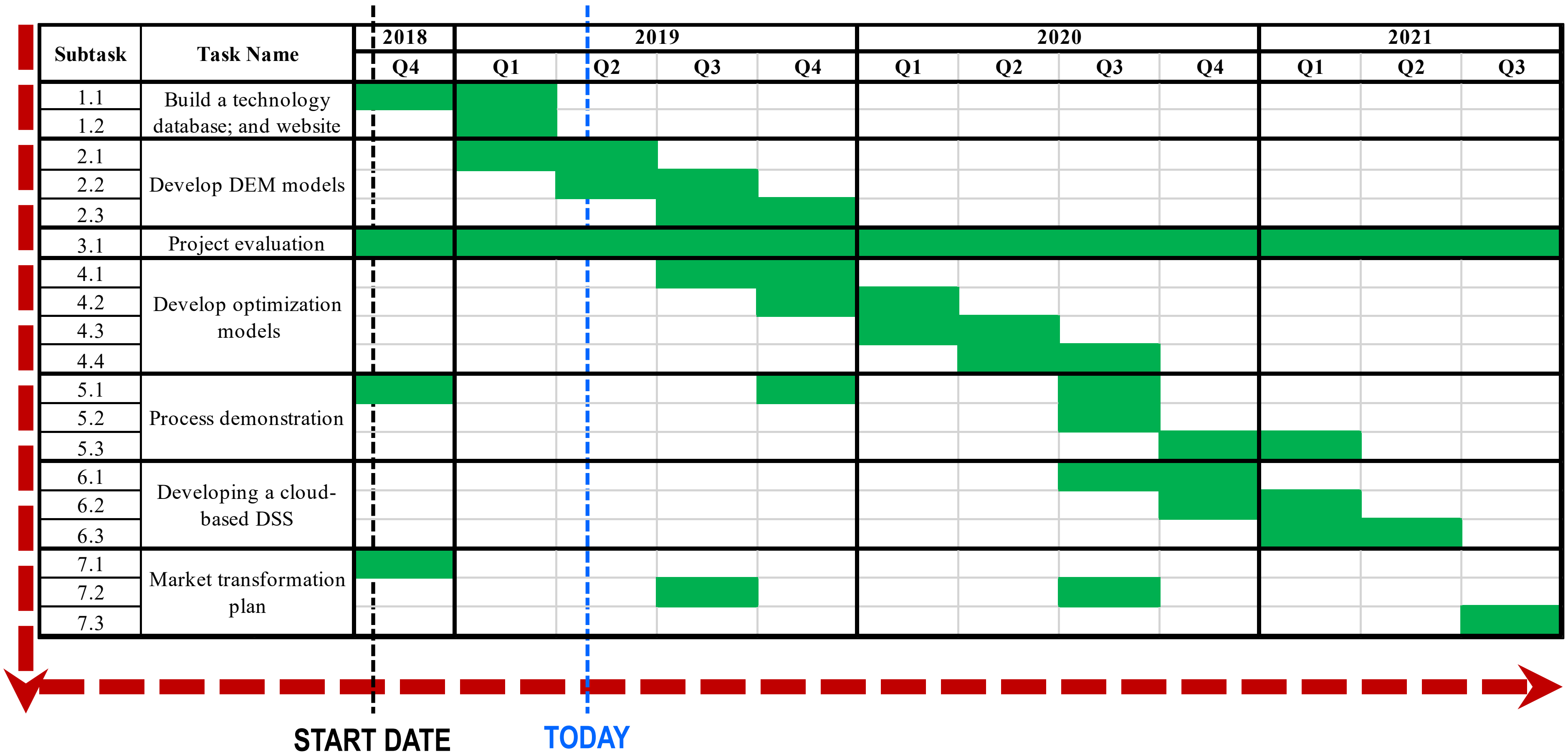
Relevance:

This research is expected to:

1. Spur the creation of a *sustainable domestic bioeconomy* by designing robust biomass feeding systems which will lead to reducing the cost of producing biofules.
2. *Enhance national biofuel production* which leads to reduced dependencies on foreign oil.

Key Milestones

Project Gantt Chart



Project Budget Table

	Original Project Cost (Estimated)		Project Spending and Balance		Final Project Costs
Budget Periods	**DOE Funding**	**Project Team Cost Shared Funding**	**Spending to Date**	**Remaining Balance**	**What funding is needed to complete the project.**
BP1 Task 1	$34,339	$3,434	$37,773	$0	$0
BP1 Task 2	$530,045	$53,005	$142,634	$440,416	$0
BP1 Task 3	$123,147	$12,315	$45,874	$89,588	$0
BP1 Task 5	$32,554	$3,255	$11,896	$23,913	
BP1 Task 7	$38,010	$3,801	$11,896	$29,915	$0
BP2 Task 2	$180,461	$18,046	$0	$198,508	
BP2 Task 3	$46,635	$4,664	$0	$51,299	$0
BP2 Task 4	$390,421	$39,042	$0	$429,464	$0
BP2 Task 5	$2,980	$298	$0	$3,278	
BP2 Task 6	$27,108	$2,711	$0	$29,819	$0
BP2 Task 7	$29,549	$2,955	$0	$32,504	
BP3 Task 3	$49,208	$4,921	$0	$54,129	
BP3 Task 5	$346,726	$34,673	$0	$381,399	$0
BP3 Task 6	$134,258	$13,426	$0	$147,684	$0
BP3 Task 7	$34,556	$3,456	$0	$38,012	$0

Quad Chart Overview

Timeline

- April 1, 2018
- March 30, 2021
- Percent complete: 15%
- Ongoing Project

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	0	0	$231,995	$1,768,004
Project Cost Share*	0	0	$18,078	$181,922

- **Partners: INL**

- ***Cost share is less than 10% of the DOE spending because of (i) the timing of graduate students hiring; and (ii) the way faculty release time is accounted for.**

Barriers

- Ft-J. Operational Reliability
- ADO-A. Process Integration
- At-B. Analytical Tools and Capabilities for System-Level Analysis

Objective

Develop *analytical tools* to enable a biorefinery to identify an *optimal integrated process* design that *ensures a reliable, cost-effective, sustainable, robust and continuous* feeding of biomass feedstocks in order to *achieve the design throughput* of the reactor.

End of Project Goal

Design a system which guarantees process reactor reliability of nearly 90% for infeed biomass with 10-30% moisture and 5-15% ash content.

Partners:

Clemson University; Idaho National Laboratory; University of Texas at San Antonio; Matera.

1. Project Overview

The main objective is to develop ***analytical tools*** to enable a biorefinery to identify an ***optimal integrated process*** design that ***ensures a reliable, cost-effective, sustainable, robust and continuous*** feeding of biomass feedstocks in order to ***achieve the design throughput*** of the reactor.

In pursue of this objective, our efforts will focus on these **specific aims**.

I. Develop **Discrete Element Models (DEMs)** to quantify and control the impact of physical and quality characteristics of biomass on the performance of the equipment used in the proposed feeding system(s).

II. Integrate the outcomes of DEMs into **Analytical Models** and develop solution algorithms to determine optimal screen size, feed rate, buffer capacity and location that optimize the performance of the feeding system.

III. Validate these analytical result via **demonstration at INL's Process Development Unit.**

1. Project Overview

I. Discrete Element Models (DEMs)

Objective: Develop DEMs to simulate biomass handling and assess impacts of input parameters on system performance.

Expected Outcomes of DEMs:

- A numerical model for simulating biomass handling that accounts for attributes of biomass, processing equipment, and technologies.
- Quantitative assessment of effects of biomass properties on system performance.
- Identify equipment design parameters for equipment given biomass properties and processing conditions.
- Develop functional relations (analytical models) for subsequent optimization models.

1. Project Overview

II. Analytical Models

Objective: Develop models to optimize the performance of reactor's feeding system.

Expected Outcomes of Mathematical Models:

- A comprehensive evaluation of the impacts of screen-size, particle distribution, material flowability, moisture and ash content have on the performance of the proposed system.
- A comprehensive evaluation of the impacts that biomass blending has on the performance of the system.

Expected Outcomes of Queuing Models:

- A comprehensive evaluation of the proposed process design using cost, equipment utilization, throughput, emissions, cycle time and in-process inventory;

Performance measures are: system-wide costs, GHG emissions and reactor utilization rate.

These models assume stochastic and/or deterministic parameters.

1. Project Overview

III. Demonstration at INL's Process Development Unit

Objective: Demonstrate the reactor maintains its reliability to nearly 90% for biomass with 10-30% moisture and 5-15% ash contents for 2 weeks.

- **Planned Feedstocks**
  – Corn stover
  – Switchgrass
  – Miscanthus

- **Feedstock standard**
  –10%-30% level of moisture
  – 5%-15% level of ash content

- **QA/QC process:**

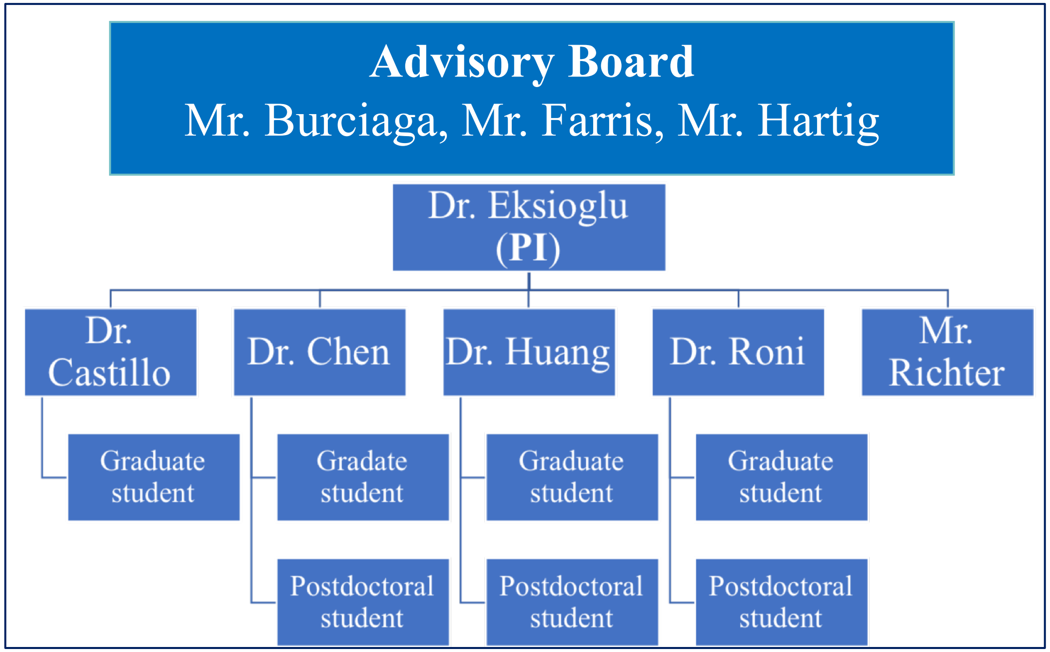
Inspect each bale to measure

- Moisture and Ash

Process Information

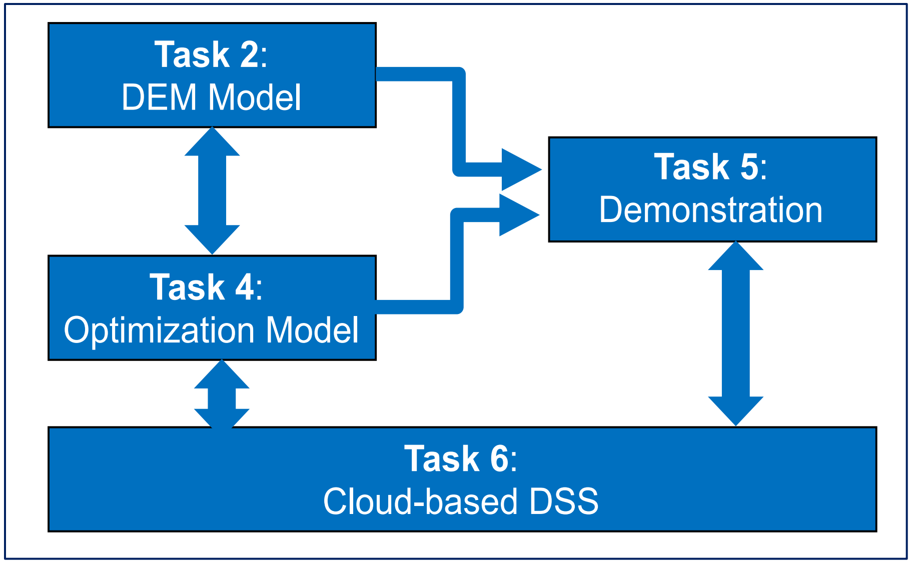
Component	Three-Pass and Two-Pass Corn Stover
Stage 1 Grinder	
Grinder type	Hammer mill
Screen Size	3 inch
Energy	16 kWh/dry ton
Capacity	2.76 ton/hour/machine
Operating conditions	25% moisture
Separations	
Screen type	Disk screen
Energy	Minimal electricity
Capacity	5 ton/hour/machine
Operating conditions	22.5% moisture
Stage 2 Grinder	
Grinder type	Hammer mill
Screen Size	1/4 in.
Energy[a]	24.7 kWh/dry ton
Capacity[a]	3.32 ton/hour/machine
Operating conditions	22.5% moisture
Densifier	
Densifier type	Pellet mill
Energy[b]	80 kWh/dry ton
Capacity	5 ton/hour/machine
Operating conditions	19.5% moisture
Dryer	
Dryer type	Cross flow grain dryer
Moisture removed	5%
Drying energy	50 kWh/dry ton
Capacity	5 ton/hour/machine

2. Approach (Management)



Organizational Chart

Process Integration



2. Approach (Management)

The **project team** includes **two** universities, **one** national lab, and **one** company.

Management Approach

1. Monthly conference calls/webinars of the team with the Technical Manager, Project Monitor and ***Advisory Board***.
2. Quarterly assessment of milestones using PMP.
3. Bi-weekly conference calls/webinars of the team.
4. Task-specific conference calls and weekly internal meetings with students and faculty.

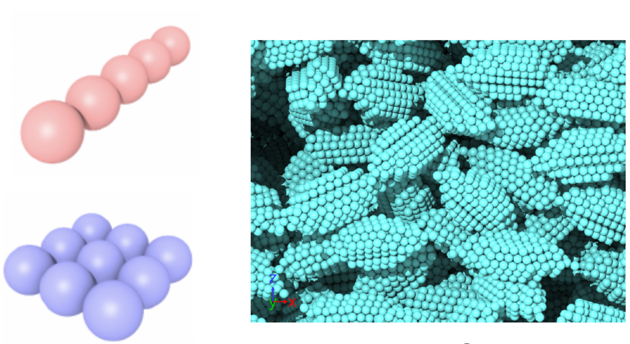
Responsibilities

Task	% Effort	Leader	Role	Support	Role
1	10	Dr. Eksioglu	Lead the development of website and review of the literature.	Dr. Castillo	Review the literature.
2	20	Dr. Chen	Lead the development and testing of DEM models.	Dr. Huang	Validate/verify DEM models.
3	5	Dr. Eksioglu	Prepare quartely and annual reports. Organize meetings.	Mr. Richter	Coordinate annual meetings.
4	20	Dr. Eksioglu	Lead the development and testing of mathematical models.	Dr. Roni	Validate/verify mathematical models.
5	25	Dr. Roni	Lead the testing the technology at INL's PDU.	Dr. Tumuluru Mr. Yencey	Coordinating the purchase of biomass.
6	15	Dr. Castillo	Lead the developing the decision support system.	All	Validate/verify the DSS.
7	5	Mr. Richter	Establish an assessment team. Conduct market transsformation analysis.	Dr. Eksioglu	Coordinate project assessment.

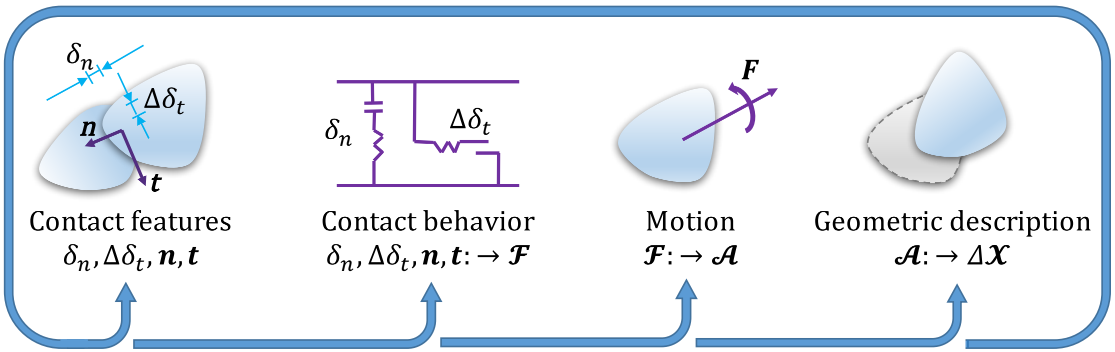
Task 2: Discrete Element Method (DEM)-based numerical models to predict material flowability and equipment performance for different feedstock types.

Methodology:

- Bonded-sphere DEM model to capture complex particle shapes, realistic size distribution, and particle deformability
- Open-source DEM code LIGGGHTS 4.0 with parallel computing for large particulate systems, run on Palmetto (Clemson) & Falcon (INL) high-performance computing clusters



Bonded-sphere model for complex-shaped deformable particles



A typical DEM computation cycle

2. Approach (Technical)

Task 4: Analytical Models for system optimization

Successive/hierarchical optimization

Step 1: Identify optimal process variables, namely screen size of grinder and separator, feed rate that contribute to (a) reduction of fine particles (b) improvement of flowability properties.

Step 2: Identify optimal buffer location, buffer size in the proposed system to achieve 90% of reactor's designed throughput considering variations of biomass quality (ash, moisture), particle size and flowability.

Step 3: Develop integrated process optimization strategy for multiple feedstocks targeting to meet biochemical conversion feedstock specs (carbohydrate 59%, ash 5%) and achieves the 90% of designed throughput of reactor.

2. Approach (Technical)

Task 5: Model validation via demonstration

Data to be gathered

- **System Reliability:**
  - Continuous run time of the proposed feeding systems.
    - A reliability level of 90% for biomass with 10%-30% moisture levels and 5%-15% ash content of proposed feeding system

- **Process performance data:**
  - Cost of optimal buffer location, buffer size in the proposed system to achieve 90% of reactor's designed throughput.
  - Cost of achievable percentage of system's designed throughput.

3. Technical accomplishments (DEM)

DEM model verification and parameter calibration

- Verification with analytical solutions for compression and bending
- Calibration for pinewood chips completed (leverage FCIC effort)
- Calibration for switchgrass ongoing

DEM process modeling 1: Hopper flow

- Influence of biomass characteristics (e.g., shape, size, stiffness)
- Influence of equipment parameters (e.g., hopper opening width, wall velocity, thickness)
- Analytical models (stress, flow rate) fitted using DEM

DEM process modeling 2: screw conveyor

- Influence of equipment parameters ongoing
- Influence of biomass characteristics ongoing

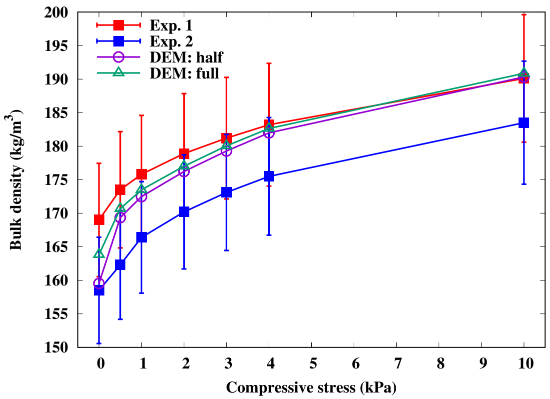
Models of PDU equipment

- Obtained all PDU equipment measurements
- Computer-aided design (CAD) drawings and DEM models in development

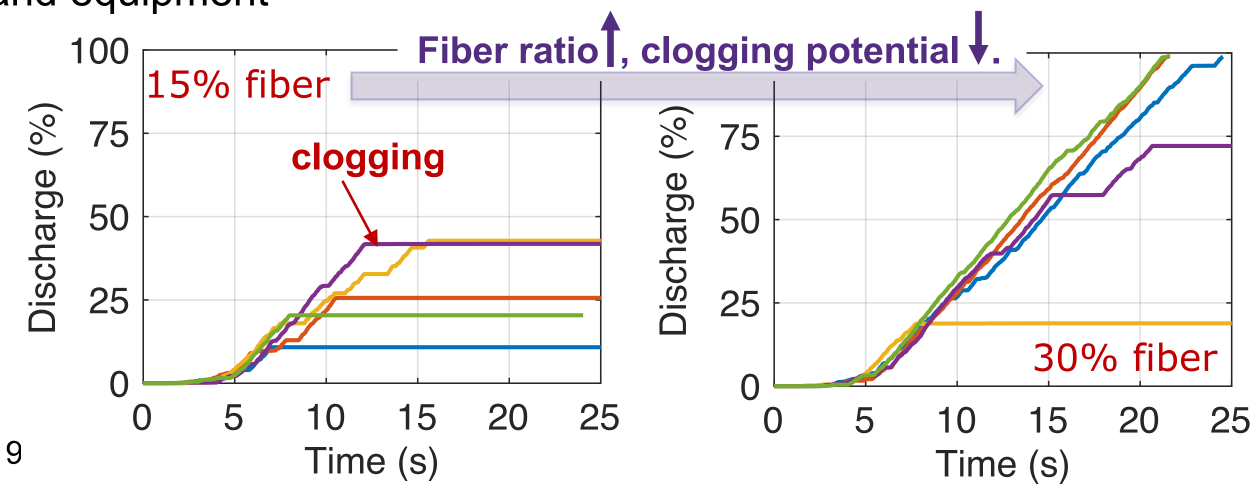
3. Technical accomplishments

DEM parameter calibration and process modeling (hopper flow)

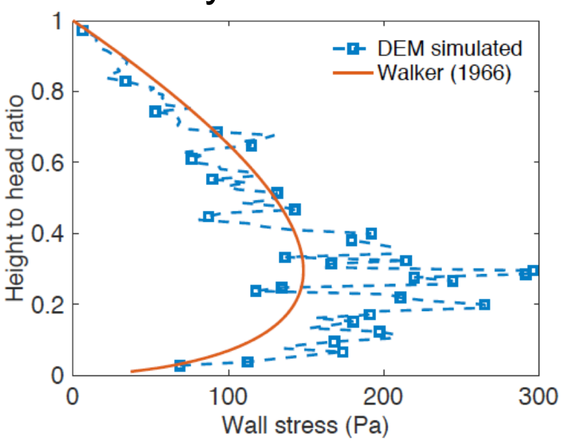
- Parameter calibrated for woodchips (leverage FCIC material handling task)
- Biomass characteristics and equipment



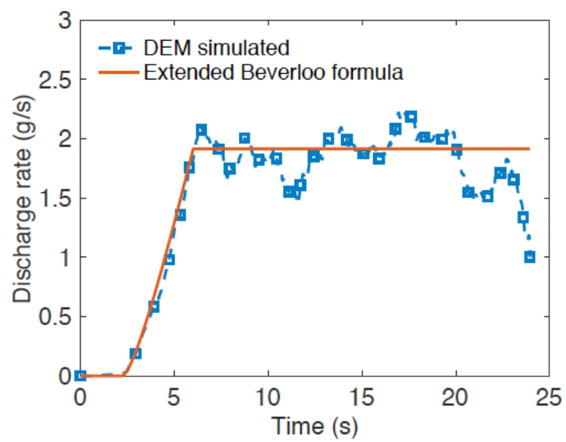
Bulk density vs. stress (Xia et al. 2019



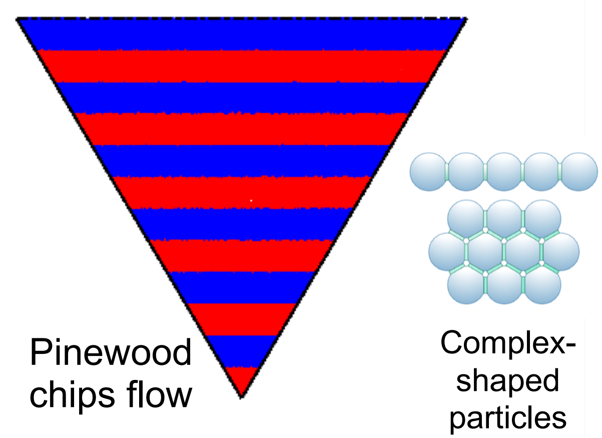
- Analytical models fitted using DEM simulations



$$\sigma_n = D\bar{\sigma}_v \frac{1 + \sin\phi \cos 2\beta}{1 - \sin\phi \cos 2(\alpha + \beta)}$$



$$W_B = C\rho_b \sqrt{g}(D_0 - \lambda d)^{2.5}$$



4. Relevance

- Our **goal** of developing a feeding system design – from biomass grinding to the reactor throat – which ensures reactor reliability nearly 90% for biomass with 10-30% moisture and 5-15% ash contents **contributes to improving process reliability**
  - Barrier Ft-J. Operational Reliability.

- The **analytical models** we propose to determine optimal screen size, feed rate, buffer capacity and location **contribute to optimizing the performance of the feeding system.**
  - Barrier ADO-A. Process Integration
  - Barrier At-B. Analytical Tools and Capabilities for System-Level Analysis

4. Relevance

Tech transfer/market plan

I. **Engage the Advisory Board** to ensure our project is relevant to the industry:

- We meet regularly (monthly) to discuss assumptions we make, methods used, guide the applicability of the research conducted, and corroborate with experiences.

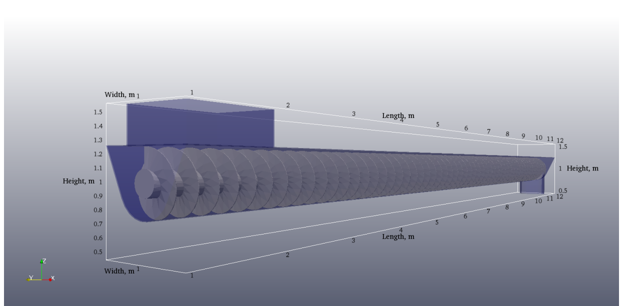
II. **Market Reception** analysis to outline investment potentials/risks

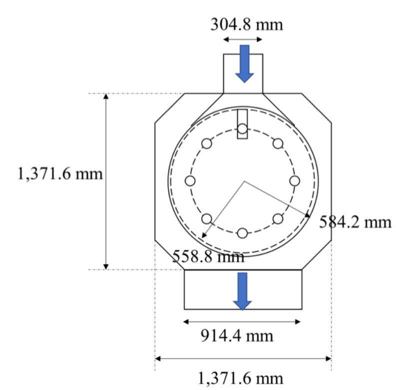
- Upon completion, this project will be presented to investment banks and equity sponsors who have taken positions in biomass conversion with a goal of understanding the investor concerns of biomass handling at commercial rates.
- We will summarize the findings via a Market Reception report with be developed based on recommendations made by investors. This report will outline recommendations on areas of concern or additional risk identified by the research efforts.

Task 2: DEM Modeling

- **DEM Model Development**
  - Parameter calibration for switchgrass, corn stover, and miscanthus
  - Extensive sensitivity studies to support analytical model developments
  - Implicit modeling of moisture and fine contents through constitutive laws (particle-particle cohesion)
- **System Performance**
  - Performance evaluation for biomass in PDU units (screw conveyor, drag conveyor, grinder, metering bin)
  - Numerical model to analytical model for system optimization
- **Other Future Plan**

Screw conveyor-1





Grinder-2

5. Future Work

Task 4: Analytical Models for system optimization

Successive/hierarchical optimization

Step 1: Develop non-linear optimization model to identify optimal process variables

- **Objective function**: minimize fine particles, maximize flowability properties
- **Decision variables**: screen size of grinder and separator, feed rate, conveyor speed etc.
- **Constraints**: variability feedstock physical properties such as followability, particle size, etc.

Step 2: Develop math models to identify optimal buffer location/size

- **Objective function**: minimize expected costs
- **Decision variables**: buffer location, buffer size
- **Constraints:**
  - Mass balance based on feed rate, conveyor speed, flowability, etc.
  - System reliability (also known as chance constraints)

5. Future Work

Task 4: Analytical Models for system optimization

Step 3: Develop stochastic, non-linear optimization model for a blending scenario with multiple feedstocks targeting to meet biochemical conversion specks

- **Objective function**: minimize costs
- **Decision variables**: the number of parallel lines/trains needed
- **Constraints:**
  - Meet conversion specs
  - Mass balance based on feed rate, conveyor speed, flowability, etc.
  - System reliability (also known as chance constraints)
  - Meet feedstock demand of the reactor

Summary

Overview: The **goal** is to reduce the cost of producing biofuels by designing a reliable, cost effective, sustainable, robust system for feeding of biomass feedstocks to the reactor.

Approach: We are developing **Discrete Element Models (DEM)** to quantify and control the impact of physical and quality characteristics of biomass on the performance of the equipment used. The outcomes of DEMs will be integrated with **Analytical Models** to determine optimal screen size, feed rate, buffer capacity and location that optimize the performance of the feeding system.

Accomplishments: We are currently working on (i) DEM model verification and parameter calibration of switchgrass; (ii) DEM process modeling of hopper flow and screw conveyor.

Relevance: This research, by will contribute to the creation of a sustainable domestic bioeconomy by designing robust biomass feeding system that leads to reduced cost of biofuel.

Future Work: (i) Continue developing the DEM model; (ii) Develop the analytical models; (iii) Validate analytical models and results via **demonstration at INL's Process Development Unit.**

Acknowledgements

- *Acknowledgements*

Additional Slides

Project Risks and Mitigation Strategies

Name	Status	Target Completi on Date	Severity	Response	Description
Incorporating the effect of temperature on feedstock handling in DEM modeling.	Known	Q3, Year1	Medium	Mitigate	There is no straightforward way, in the D framework, to model the frictional heat a subsequently, heat dissipation and moistu To model the particle flow (DEM) and co heat-moisture transport in the system, the approaches in fluidized beds could be bo In which, one coupled use CFD for fluid mass/heat transport in voids (between DE particles) and do CFD-DEM coupling.
Lack of availability of input data for validation.	Known	Q1, Year1	Medium	Mitigate	This project relies on data availability fro related R&D projects for simulation mod validation. If new data for different feeds components in a blended feedstock is not available on time, data from feedstock wi properties will be utilized.
DEM simulations are computational intensive.	Unknown	Q4, Year1	Medium	Accept	DEM simulations of many particles and continuum-type simulations have high de freedom with non-linear properties, whic likely lead to model stability challenges.
Feedstock supply uncertainty	Known	Q4, Year2	Medium	Mitigate	Miscanthus and Switchgrass will be much difficult to bring in, as they are both inva species. They are not widely used comme Based on availability of feedstock, proces demonstration scenario will be selected.
Validating analytical results	Known	Q2, Year3	Medium	Mitigate	The proposed process for demonstration high moisture pelleting. This is a new pro achievement of the performance metrics PI/Co-PI will keep track of ongoing lab- and pilot scale experiments at INL to pre ability to scale-up to a commercial scale and achieve the performance metrics
Integrating incompatible analytical model in DSS	Known	Q1, Year3	High	Mitigate	DSS will couple various analytical mode Integration of various models is challeng output-input data connections will be alig produce meaningful results.

Publications and Presentations

Publications

•Y. Xia, Z. Lai, T. Westover, J. Klinger, H. Huang and Q. Chen, “Discrete element modeling of deformable pinewood chips in cyclic loading test”, Powder Technology, 345: 1-14, https://doi.org/10.1016/j.powtec.2018.12.072, (2019).

•Z. Lai, Y. Xia, H. Huang, T. Westover and Q. Chen, “Discrete element modeling of granular hopper flow of irregular-shaped deformable particles”, Powder Technology, in review, (2019).

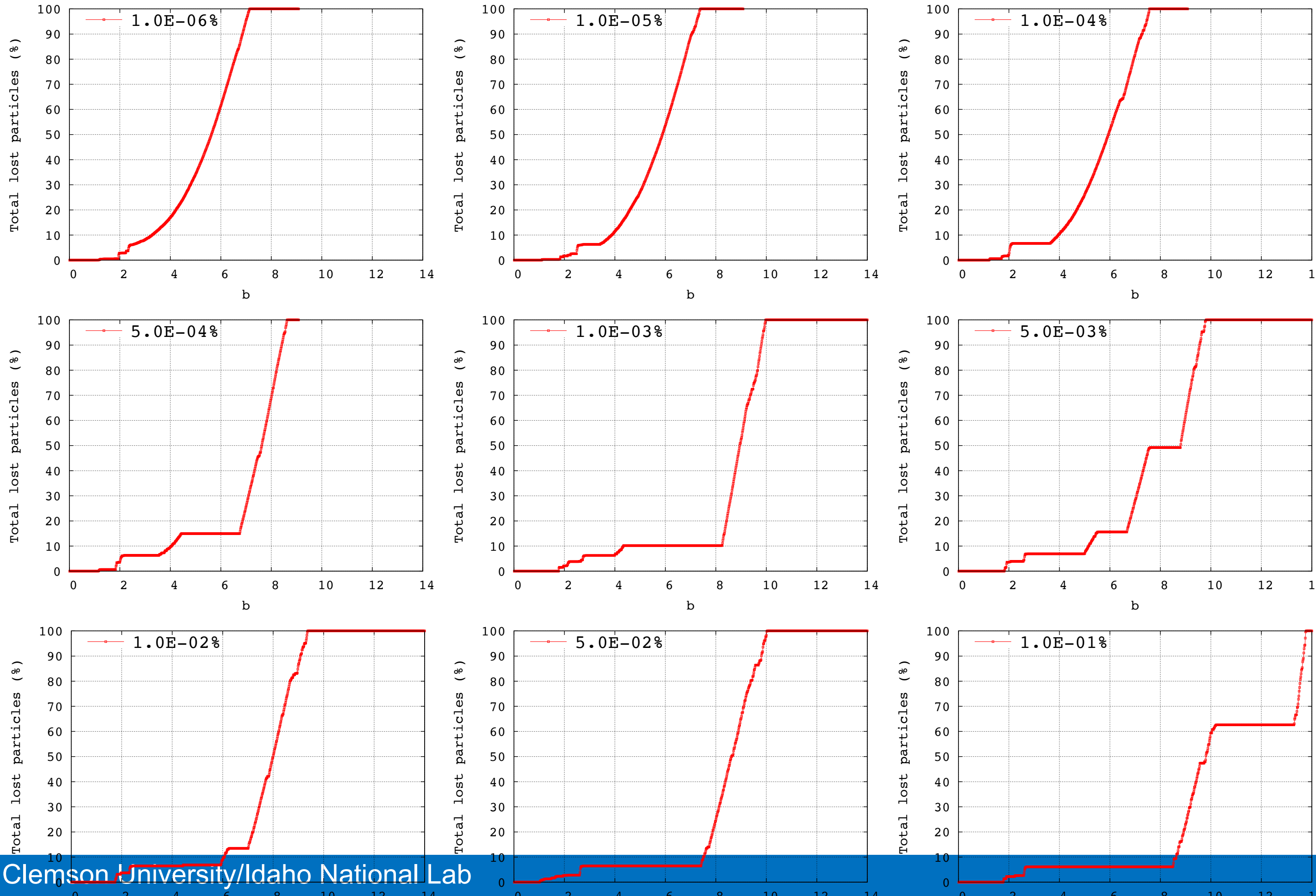
Presentations

•Z. Lai, Y. Xia, H. Huang, T. Westover and Q. Chen, “Numerical characterization of biomass flowability in biorefinery”, Idaho National Laboratory Annual Intern Expo, Idaho Falls, ID, (2018).

Previous and On-Going Research Efforts

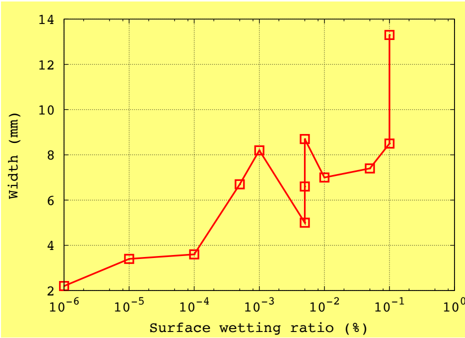
Feedstock supply and logistic – Led by INL

DEM simulation of hopper flow with varying moisture content



b = hopper opening width (mm) / particle diameter (1mm)

13179 total particles



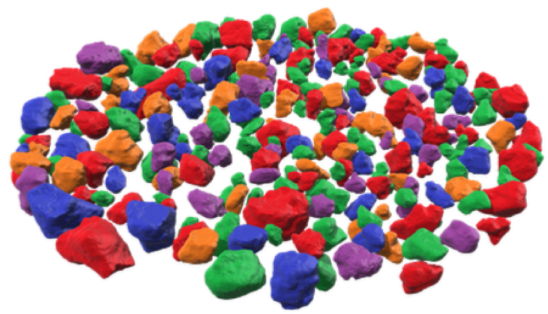
Hopper opening width (when continuous particle flow starts) versus. particle surface wetting ratio

Previous and On-Going Research Efforts

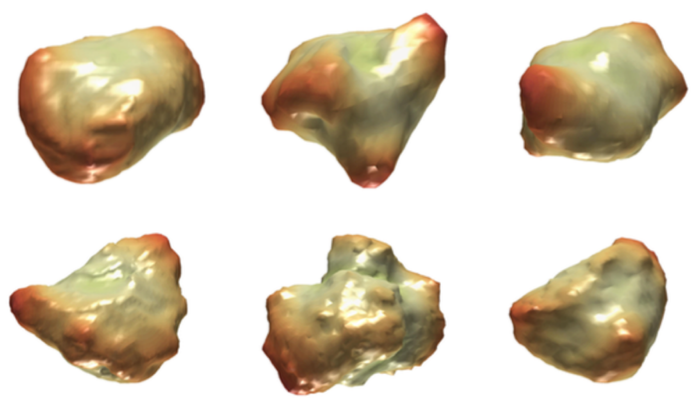
Computational mechanics research – Clemson

Characterize Morphology of Arbitrary Shaped Particles

Particle of arbitrary shapes



Particle reconstruction from X-ray CT



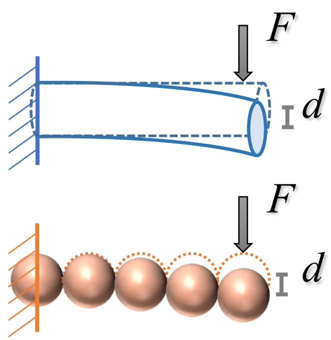
Characterize particle shape descriptors:

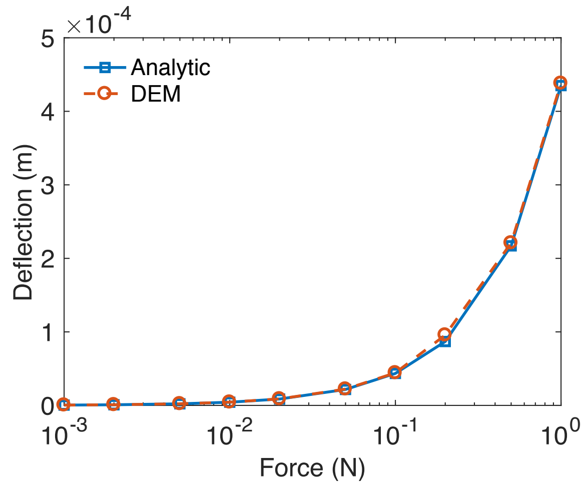
- dimensions, form, sphericity, roughness

DEM Verification

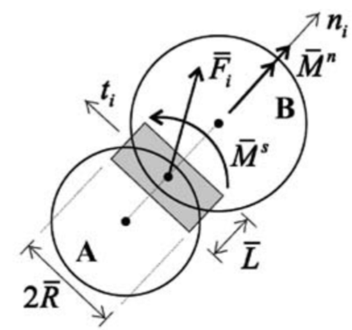
DEM model verification: DEM linear parallel bond model

- Bending test of cantilever beam

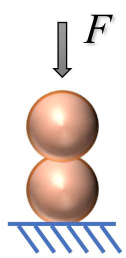


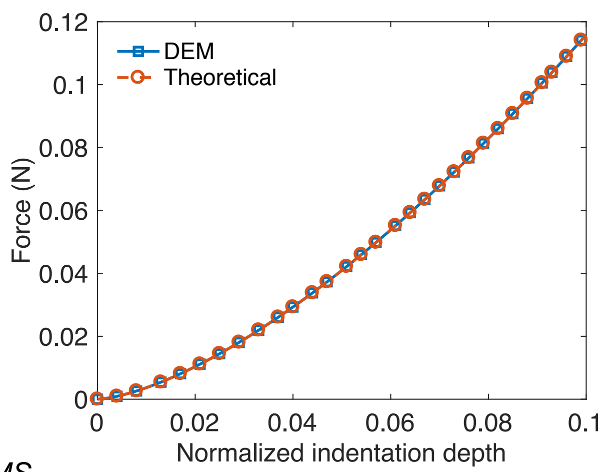


From (Potyondy & Cundall, 2004)



- Axial compression of cantilever beam





$$\Delta F^n = k_b^n A \Delta U^n$$

$$\Delta F^s = -k_b^s A \Delta U^s$$

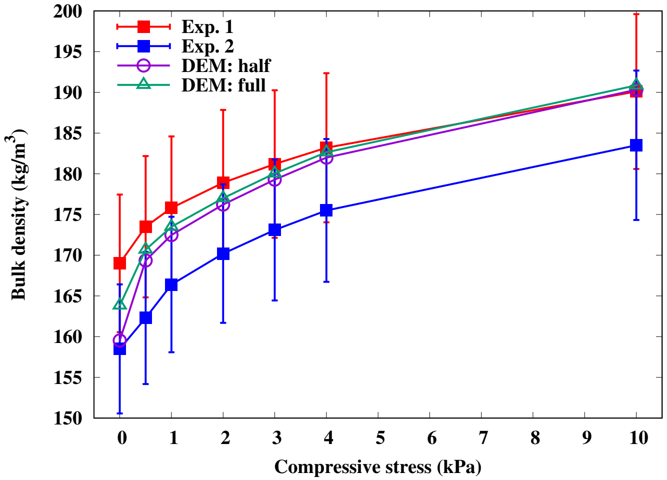
$$\Delta M^n = -k_b^s J \Delta \theta^n$$

$$\Delta M^s = -k_b^n I \Delta \theta^s$$

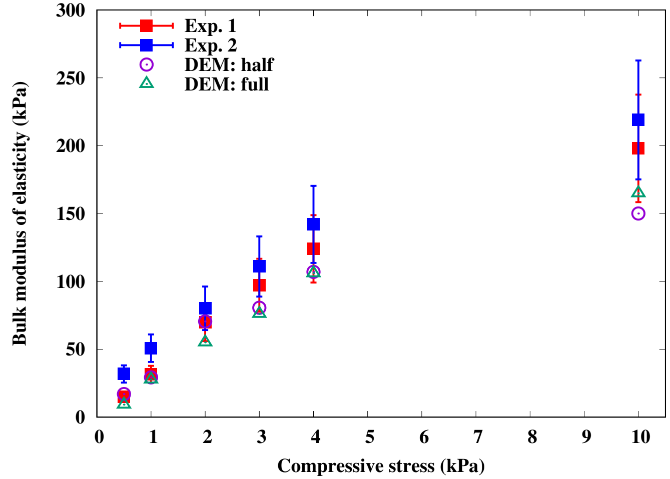
[1] Potyondy, D. O., & Cundall, P. A. (2004). *IJRMMS*.

DEM Parameter Calibration

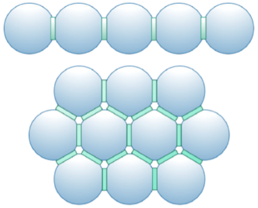
Model calibration (pinewood chips, FCIC)



Bulk density vs. stress (Xia et al. 2019)



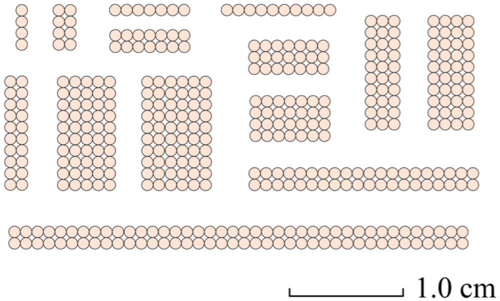
Bulk modulus vs. stress (Xia et al. 2019)

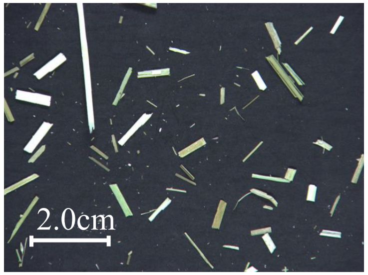


DEM: fiber & plate

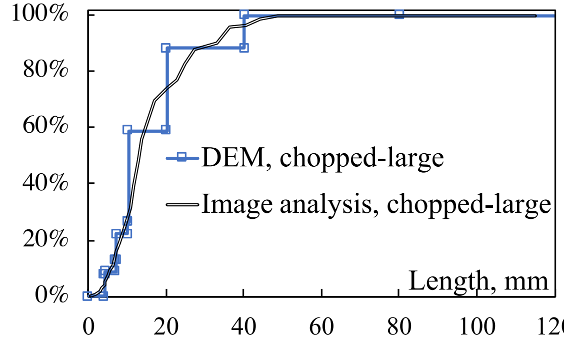
Model calibration (switchgrass, ongoing)

- Switchgrass characterization at INL (Westover et al. 2015)

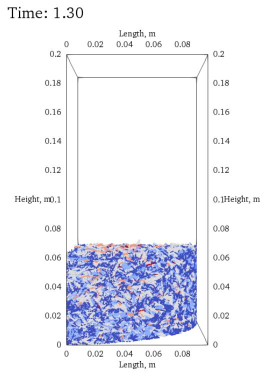




Particle shapes
DEM vs. image analysis



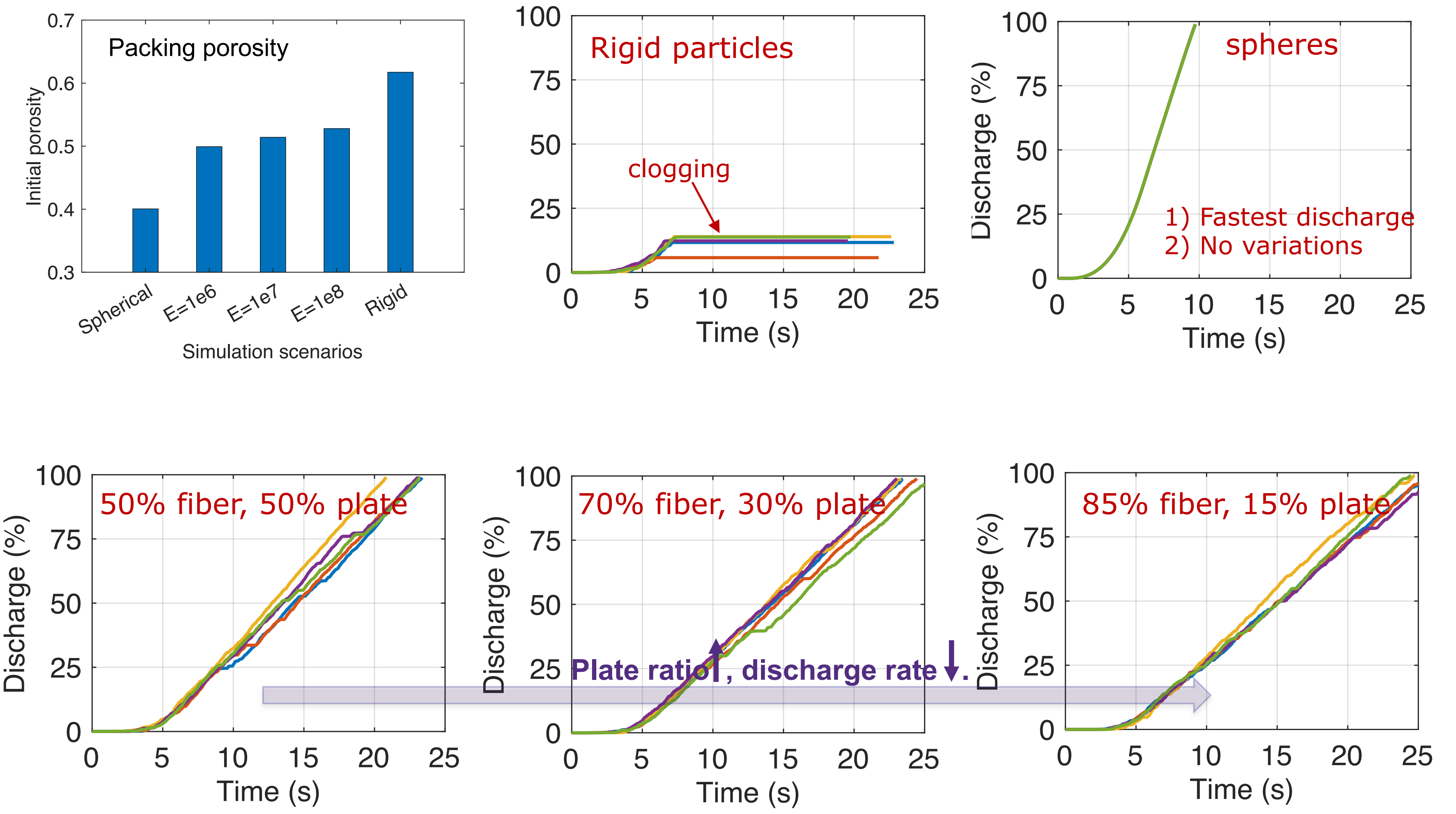
Particle size distribution
DEM vs. image analysis



Compression test

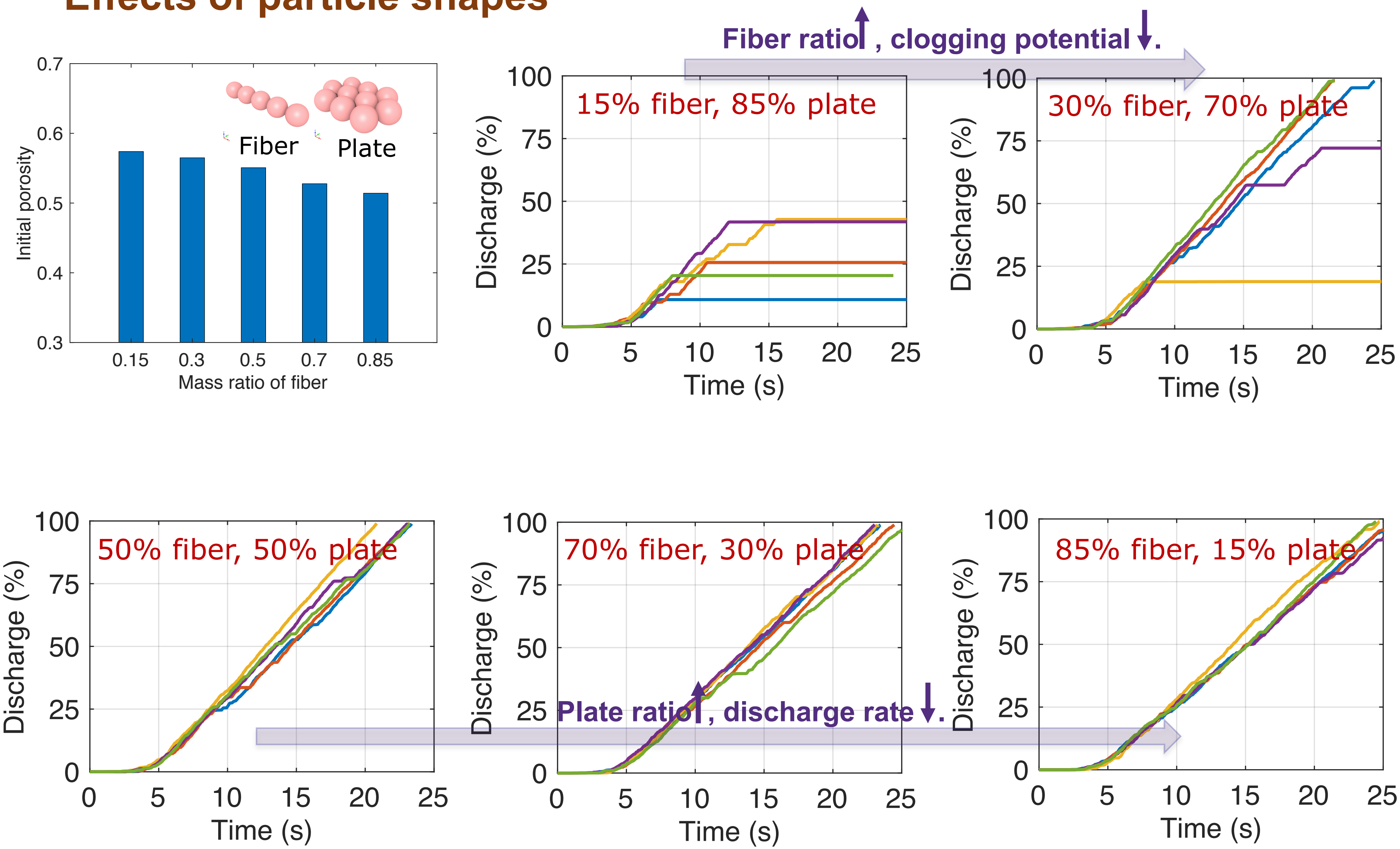
DEM Hopper Flow Simulations

Effects of particle stiffness



DEM Hopper Flow Simulations

Effects of particle shapes

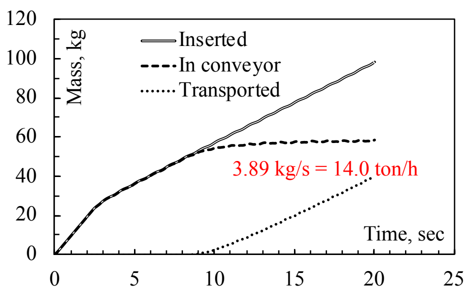


DEM Screw Conveyor Simulations

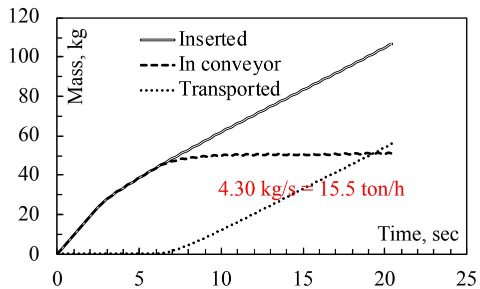
DEM process modeling 2: screw conveyor flow

- Quantitative analysis on effect of equipment settings and biomass characteristics on flow behavior (ongoing)

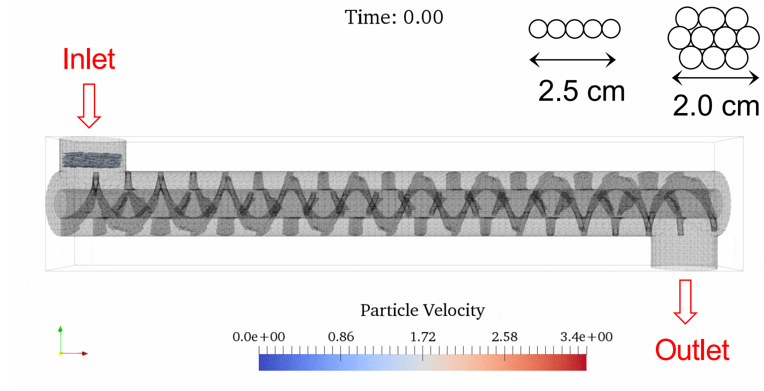
Rotational speed: 60 rpm



Rotational speed: 90 rpm

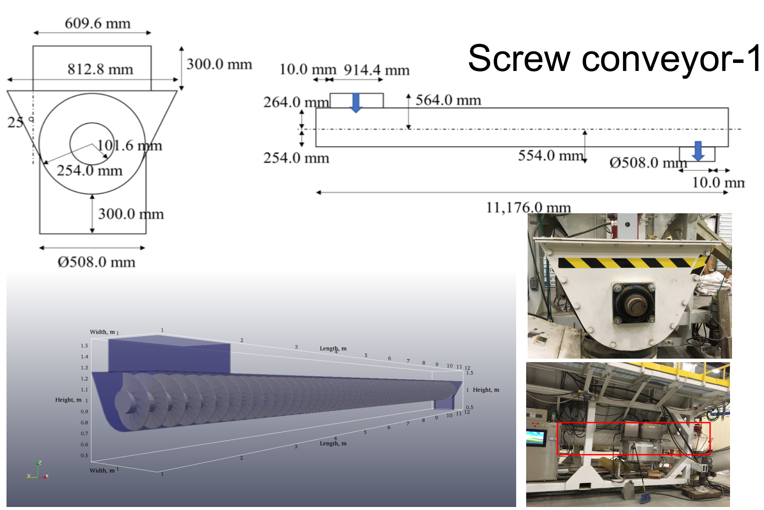


- Transport rate increases with rotational speed.

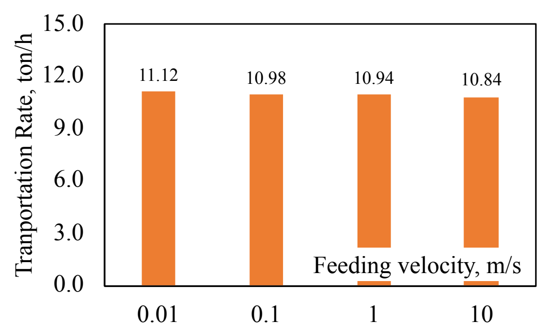


- Screw conveyor length of 5.0m, diameter of 0.5m
- Around 2,000,000 base spheres

Models of PDU units



Sensitivity study on feeding velocity

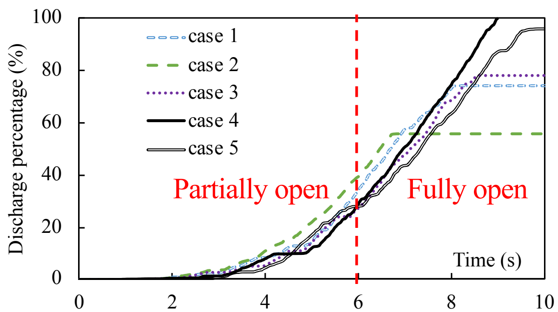


- No significant influence

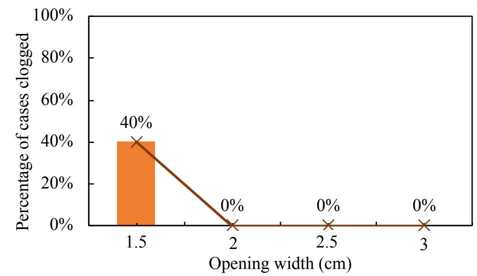
Rigid Hopper Flow

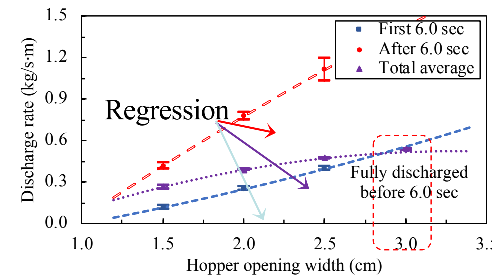
- Hopper flow model with rigid particles
  - Palmetto HPC
  - Sensitivity study on particle size, orifice size, and Fiber/Plate ratio

- Different realizations

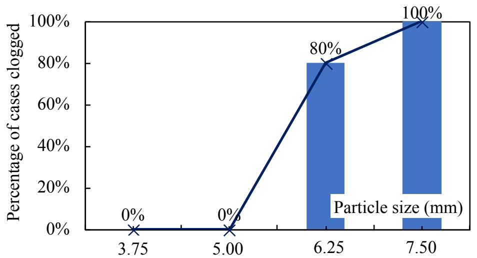


- Orifice size



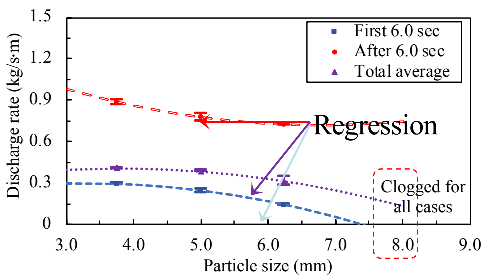


- Particle size

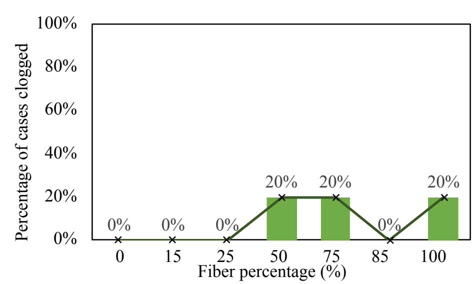


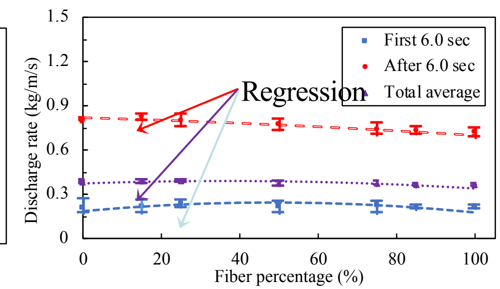
Fiber:

Plate:



- Fiber/Plate ratio





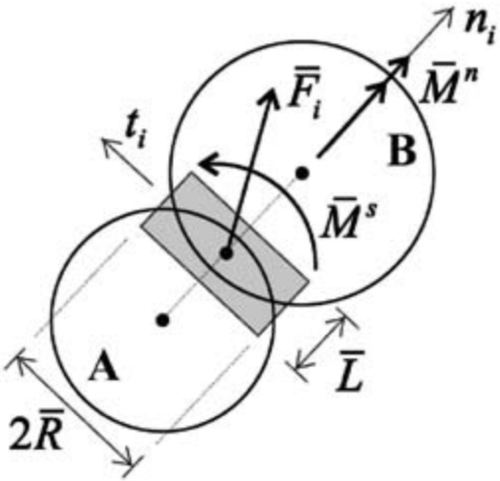
$$Average\ flow\ rate = 0.12d_p - 0.02d_p^2 + 0.53d_{ori} - 0.08d_{ori}^2 + 0.08FPR - 0.11FPR^2 - 0.56$$

$$First\ 6.0\ sec\ flow\ rate = 0.12d_p - 0.02d_p^2 + 0.16d_{ori} + 0.03d_{ori}^2 + 0.25FPR - 0.26FPR^2 - 0.39$$

$$After\ 6.0\ sec\ flow\ rate = -0.25d_p + 0.02 + 0.88d_{ori} - 0.05d_{ori}^2 - 0.07FPR - 0.04FPR^2 + 0.03$$

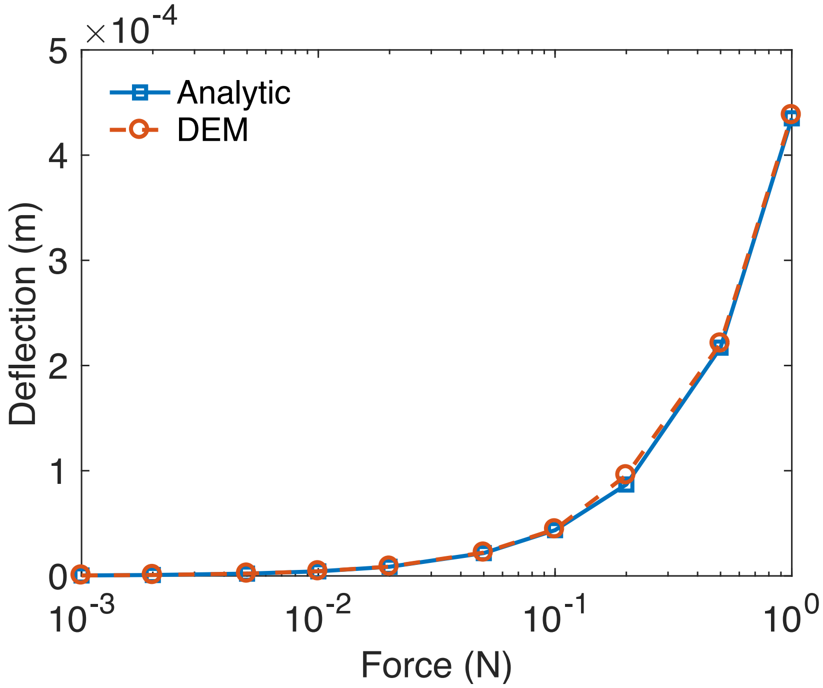
Deformable Particle Contact Model

- Linear Parallel Bond Model



$$\Delta F^n = k_b^n A \Delta U^n$$
$$\Delta F^s = -k_b^s A \Delta U^s$$
$$\Delta M^n = -k_b^s J \Delta \theta^n$$
$$\Delta M^s = -k_b^n I \Delta \theta^s$$

A, I, J are the area, moment of inertia and polar moment of inertia of the bond.



1. Potyondy, D. O., & Cundall, P. A. (2004). *IJRMMS*.

Inter-particle Contact Model

- Hertz-Mindlin contact model

$$F = (\underbrace{k_n \underbrace{\delta n_{ij}}_{\text{normal overlap}} - \gamma_n \underbrace{vn_{ij}}_{\text{normal relative vel.}}}_{\text{normal force}}) + (\underbrace{k_t \underbrace{\delta t_{ij}}_{\text{tangential overlap}} - \gamma_t \underbrace{vt_{ij}}_{\text{tangential relative vel.}}}_{\text{tangential force}})$$

The tangential overlap is truncated to fulfil $F_t \leq x_{u} F_n$

$$S_n = 2Y^* \sqrt{R^* \delta_n}, \qquad S_t = 8G^* \sqrt{R^* \delta_n}$$

$$\beta = \frac{ln(e)}{\sqrt{ln^2(e) + \pi^2}},$$

$$\frac{1}{Y^*} = \frac{(1-\nu_1^2)}{Y_1} + \frac{(1-\nu_2^2)}{Y_2},$$

$$\frac{1}{G^*} = \frac{2(2-\nu_1)(1+\nu_1)}{Y_1} + \frac{2(2-\nu_2)(1+\nu_2)}{Y_2}$$

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2}, \quad \frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2}$$

Y...Young's modulus G...Shear modulus

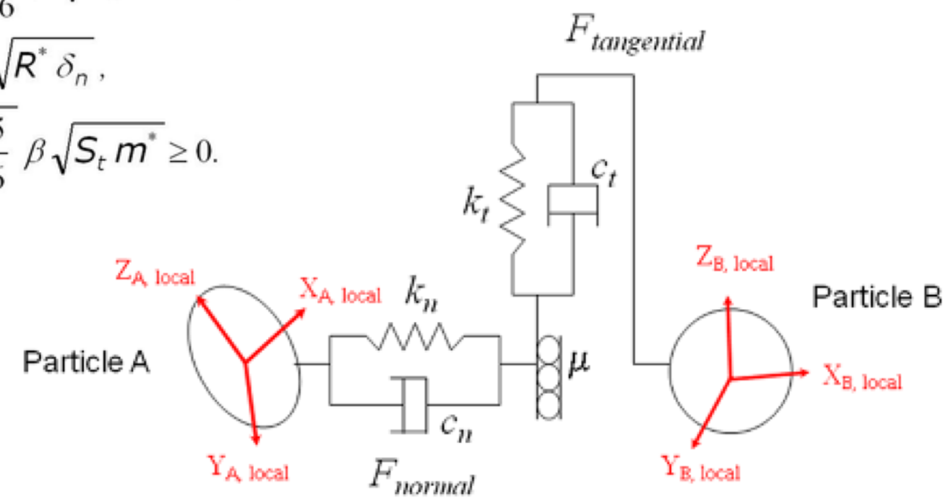
ν...Poisson ratio e...coeff.of restitution

$$k_n = \frac{4}{3} Y^* \sqrt{R^* \delta_n},$$

$$\gamma_n = -2\sqrt{\frac{5}{6}}\, \beta \sqrt{S_n m^*} \geq 0,$$

$$k_t = 8G^* \sqrt{R^* \delta_n},$$

$$\gamma_t = -2\sqrt{\frac{5}{6}}\, \beta \sqrt{S_t m^*} \geq 0.$$



1. Di Renzo, A., & Di Maio, F. P. (2005). *Chemical engineering science*.
2. https://www.edemsimulation.com.