DOE Bioenergy Technologies Office
2019 Go/No-Go Review (DE-EE0008255)

Integrated Process Optimization for Biochemical Conversion

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OUTLINE

1. Project Overview

Main objective:

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**.

Three specific aims:

Focus of Year 1

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.**

2. Key Milestones & Go/No-Go

MS	Description	Date
1.1	Complete a database of literature related to cutting edge technologies and input process data for modeling	Year 1 Q2
1.2	Project website is available on-line. Related publications and input process data are available through the website.	Year 1 Q2
2.1	**Complete numerical analysis to support selection of the approach used to model coupled heat-moisture transport.**	Year 1 Q3
2.2	**Complete DEM model development**.	Year 1 Q4
2.3	**DEM model verification/validation:** (i) provides (simulated) particles size distribution for each process and for each feedstock under various moisture (5%-35%) and ash contents (2%-15%) in the proposed system design; and estimates the percentage of fine particles (<1/16”); (ii) provides (simulated) flowability properties of each feedstock (e.g. rate of flow, wormhole effect) in the proposed system under various moisture (5%-35%) and ash content (2%-15%); (iii) estimates the % change of mean time to failure of each equipment in the proposed system and for each feedstock due variations in particle size distribution, moisture, ash and flowability. Equipment is in failure mode if it is not operating.	Year 2 Q1
3.1	Complete initial comprehensive project summary presentation and deliver the presentation on-line.	Year 1 Q1
3.2	Complete quarterly reports and an annual report.	Quarterly
3.3	Complete the peer review based on DOE reporting requirements.	Year 2 Q4
7.1	Establish an assessment team.	Year 1 Q1
7.2	The assessment team establishes project performance measures.	Year 2 Q2
Go/No-Go	Prediction accuracy of the DEM model will be determined via testing using historical experimental data of INL and ORNL. The performance of the DEM model will be determined based on **(a) the accuracy of the DEM model** to predict particle size distribution and flowability; **(b) the usefulness and quality of data** available at INL and ORNL. **Go:** The data provided by INL and ORNL for corn stover (other material: switchgrass) is of quality; and the model predicts accurately the particle size distribution and flowability properties of biomass in the proposed process 90% of the time. Continue the development of optimization model.	

2. Key Milestones & Go/No-Go

MS	Status / Justification	Date
1.1	**Completed.** Related data and literature have been collected.	Year 1 Q2
1.2	**Completed.** Project website is online, and related publications are available. https://cecas.clemson.edu/Integrated_Biorefinery/.	Year 1 Q2
2.1	**Completed.** The liquid-bridge model has been selected to explicitly model the effect of moisture. This model has been adopted in the DEM model and the implementation in LIGGGHTS has been verified. Numerical simulations of biomass flow under different moisture contents have been conducted to quantify the effect of moisture.	Year 1 Q3
2.2	**Completed.** Key DEM model developments: (**1**) bonded-sphere model (for complex-shaped deformable biomass particles); (**2**) sphere with rolling resistance model (for computational efficiency, while accounting for shape effect); (**3**) liquid-bridge model (for explicitly modeling moisture effect); (**4**) coarse-graining method (for upscaling to PDU equipment scale simulations); (**5**) an open-source parallel DEM code LIGGGHTS; (**6**) CAD drawings and the corresponding DEM model developed for all screw and drag chain conveyors, and hoppers in PDU.	Year 1 Q4
3.1	**Completed.** The team has completed the initial project review and delivered the online presentation.	Year 1 Q1
3.2	**Completed.** The team has submitted all required reports.	Quarterly
7.1	**Completed.** An assessment team has been established.	Year 1 Q1
2.3	**Ongoing (Year 2 Q1).** (1) The bonded-sphere model has been verified against known analytical solutions; (2) Calibration for switchgrass is completed, and comparison of DEM simulations with INL experimental data for compression and ring shear tests show the validity of the model; (3) DEM simulations of biomass flow are performed and impacts of biomass characteristics on flow through extensive sensitivity studies; (4) ongoing efforts will use new PDU test data for DEM model validation.	Year 2 Q1
3.3	**Ongoing (Year 2 Q4).** The team is preparing for the annual comprehensive project review.	Year 2 Q4
7.2	**Ongoing (Year 2 Q2).** The advisory board has been attending meetings with DOE and provide feedback.	Year 2 Q2

2. Key Milestones & Go/No-Go

Go/No-Go based on:

I. **Performance of the DEM models** to accurately predict biomass material behavior in the proposed process
   - Evaluation of DEM performance against analytical, empirical, and experimental results/data at the particle, lab, and PDU scales.

II. **The usefulness and quality of data at INL**
   - Historical data (published and unpublished)
   - New data from recent and planned experiments

OUTLINE

3.1 DEM Basics

Discrete element method (DEM) is a particle-based numerical method for modeling granular materials (initially, for geomaterials).

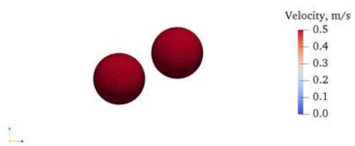
+ directly model particle collisions and interactions

+ bypass the phenomenological constitutive models

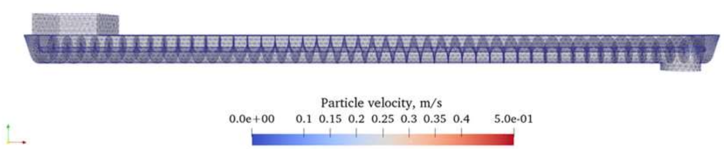
+ suitable for problems involving large deformations or material failure

- computationally very expensive

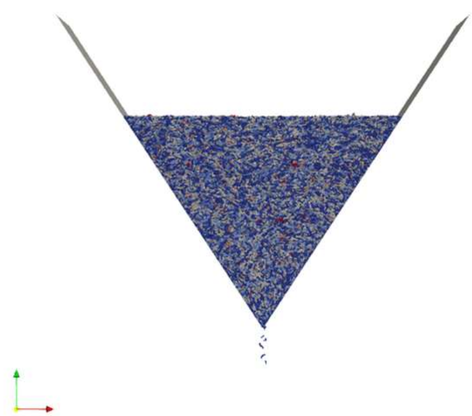
Particle collision



Screw conveyor transport



Hopper flow



Compression test

Simulations by team member Y. Guo and F. Chen

3.2 Key DEM Developments (MS 2.1&2.2)

1) Bonded-sphere DEM model

- Complexed-shaped biomass particles
- Deformable (bonded-sphere), rigid (multi-sphere)

2) Simplified sphere with rolling resistance model

- Indirectly account for the effect of irregular shapes
- Computationally more efficient

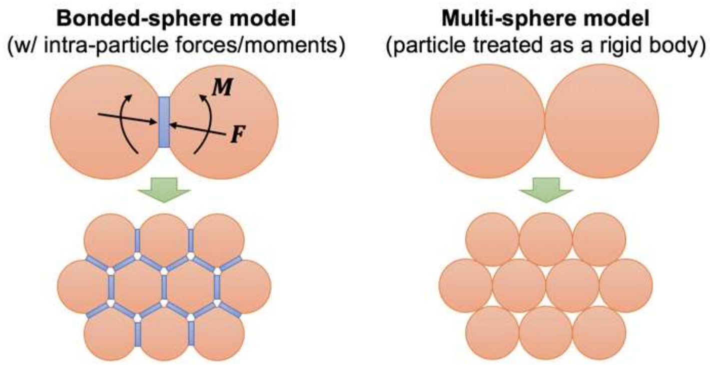
3) Liquid-bridge model

- Explicitly models the moisture effect

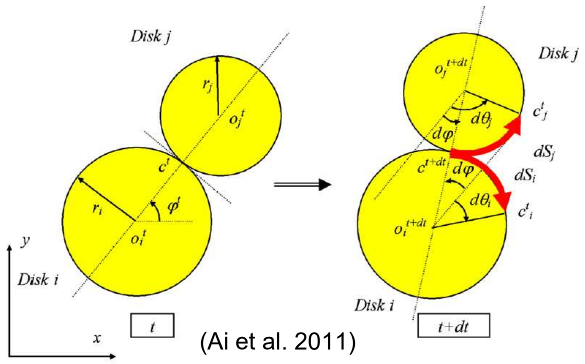
Corn stover

Switchgrass

Picture by Dr. Xia (INL)

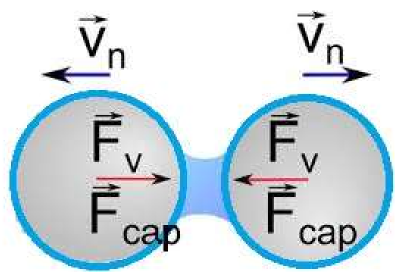


1) Bonded-sphere and multi-sphere model



(Ai et al. 2011)

2) Rolling resistance model



3) Liquid-bridge model

3.2 Key DEM Developments (MS 2.1&2.2)

4) Coarse-graining method

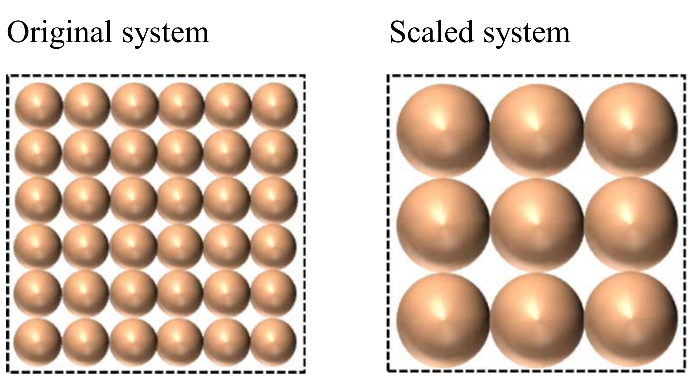
- Further improve computational efficiency
- Necessary for PDU equipment-scale modeling
- Coarse-graining laws derived

5) LIGGGHTS 4.0 parallel DEM code

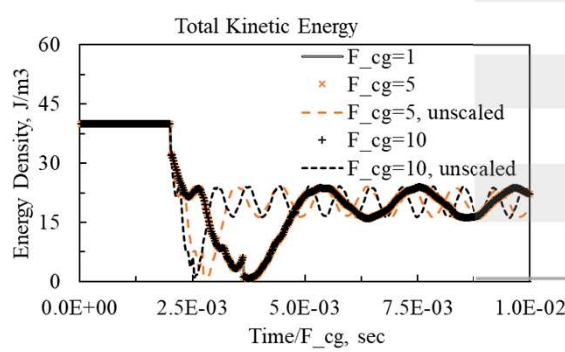
- Public version runs on Clemson's Palmetto
- Premium version runs on INL's Falcon high-performance computing clusters

Coarse-graining laws

Parameters	Factor
R'/R	F_{cg}
ρ'/ρ	1
e'/e	1
E'/E	1
ν'/ν	1
$k_n^{b'}/k_n^b$	$1/F_{cg}$*
$k_s^{b'}/k_s^b$	$1/F_{cg}$
μ'/μ	1
μ_r'/μ_r	1
σ'/σ	F_{cg}
η'/η	F_{cg}
θ'/θ	1
w_c'/w_c	1
v_p'/v_p	1
w_p'/w_p	$1/F_{cg}$
t'/t	F_{cg}



Coarse-graining method

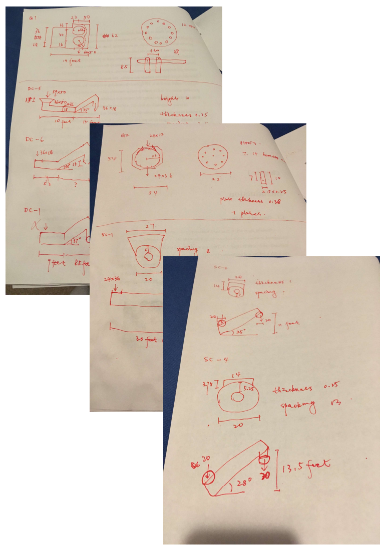


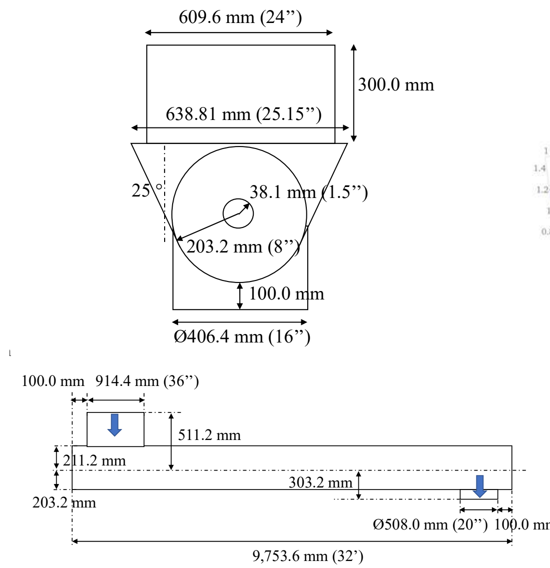
Appropriate scaling laws ensure energy consistence

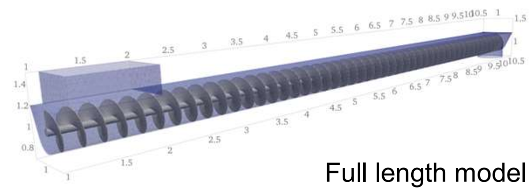
3.2 Key DEM Developments (MS 2.1&2.2)

6) DEM models of PDU equipment

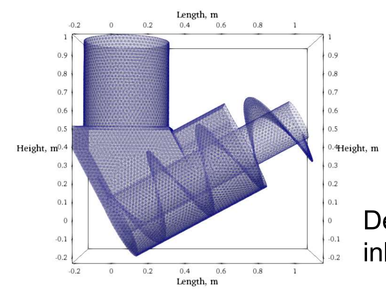
- Measurements obtained through multiple visits to PDU at INL
- DEM models developed for all key equipment







Full length model



Detailed inlet model

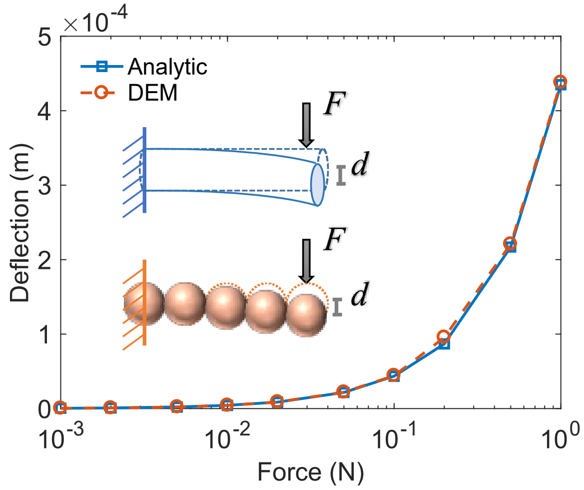
PDU equipment (SC-1 shown) ⇨ **Measurements & manual drawings** ⇨ **Computer-aided drawings (CADs)** ⇨ **DEM models (SC full and inlet models shown)**

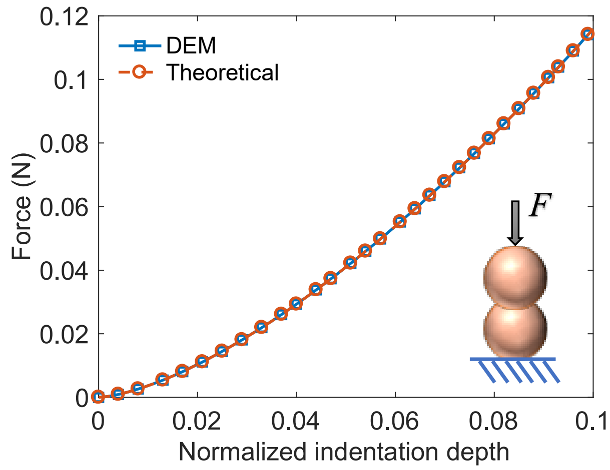
3.3 Performance Evaluation (MS 2.2 & 2.3)

No.	Test name	Purpose / Qty. of Interest / Scale	Evaluation
1	Bending & axial loading	Bonded-sphere / Force-deflection / Particle scale	Analytical
2	Collision of moisture particles	Liquid-bridge / Contact forces / Particle scale	Analytical
3	Coarse-graining collision & conveyor transport	Coarse-graining / Kinetic energy & flow / Particle & PDU scales	Energy density
4	Cyclic compression	Calib. & valid. / Mech. prop. (particle size, bulk density, stress-strain / Lab scale	Experimental
5	Ring shear	Calib. & valid. / Mech. prop. / Lab scale	Experimental
6	Hopper flow	Valid. & sensitivity / Particle flow / Lab scale	Experimental / empirical
7	Bulk density	Valid. / Biomass char. (size, moisture), bulk density / PDU scale	Experimental
8	Conveyor modeling	Valid. / Biomass char., flow/ / PDU scale	Experimental / analytical

3.3 Performance Evaluation (MS 2.2 & 2.3)

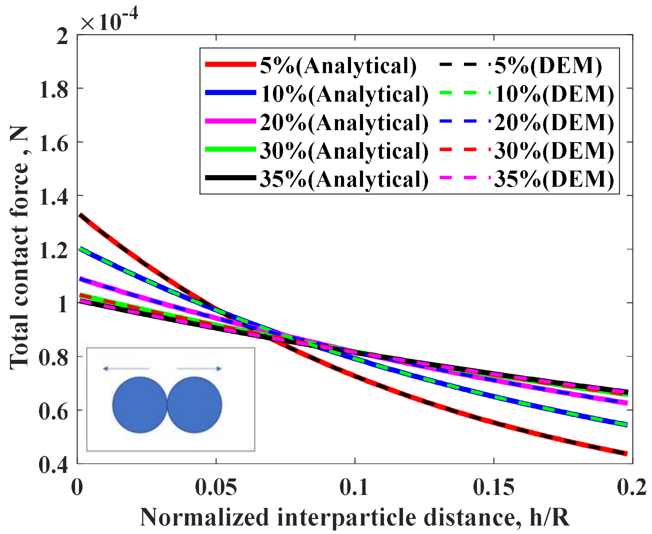
1) Bending and axial-loading tests



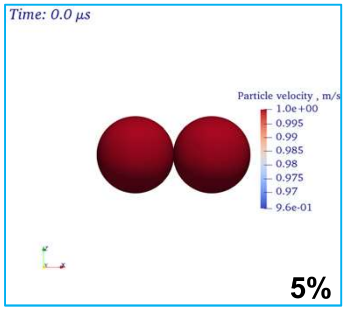


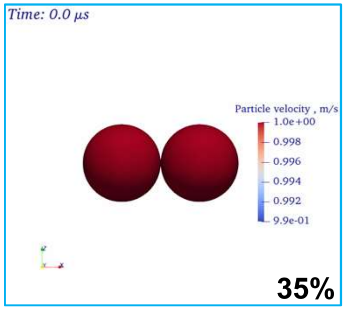
< 1% error compared to the analytical solutions

2) Collision tests of moisture particles (5% – 35% moisture)



< 1% error compared to the analytical solutions

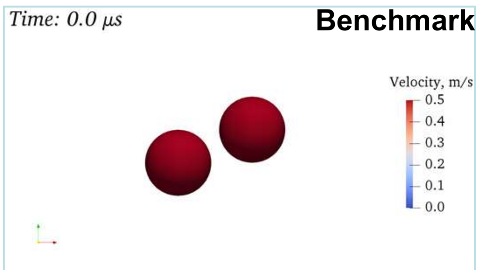


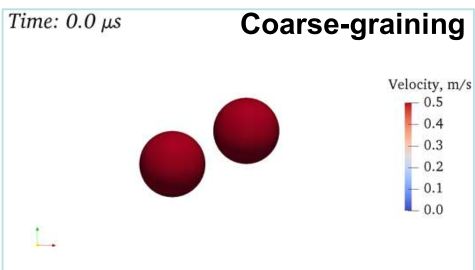


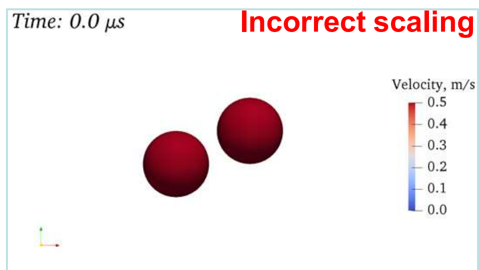
3.3 Performance Evaluation (MS 2.2 & 2.3)

3) Coarse-graining collision & transport

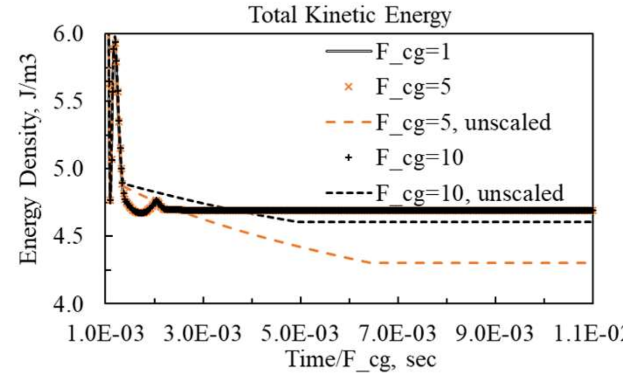
- **Case 1**: moist particle collision
- Liquid bridge + rolling resistance + Hertz-Mindlin

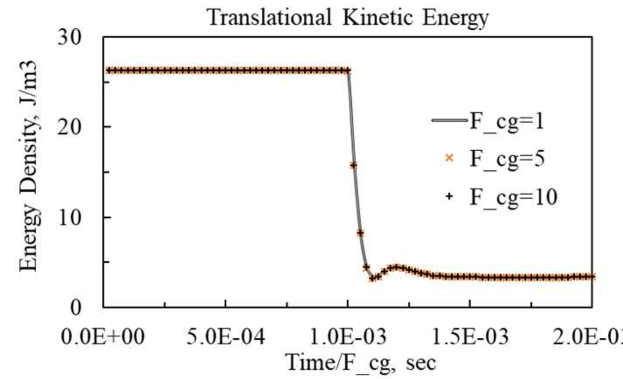


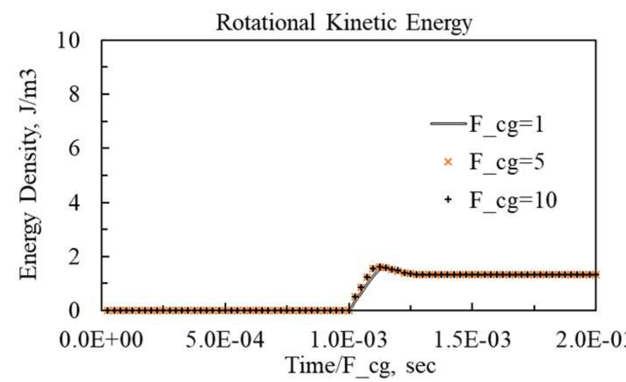




Coarse-graining has **<u>< 1%</u>** error (total kinetic energy) compared to the benchmark (F_cg=1) both during and after the collision.





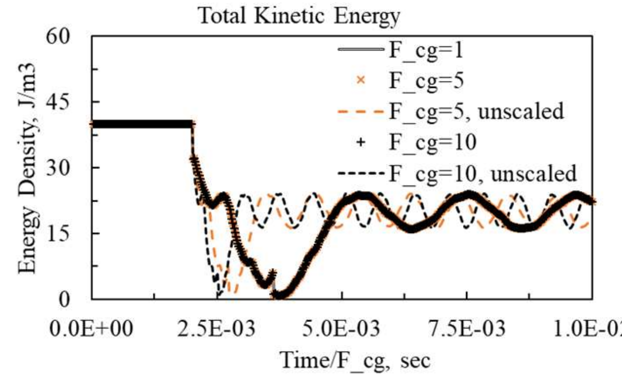


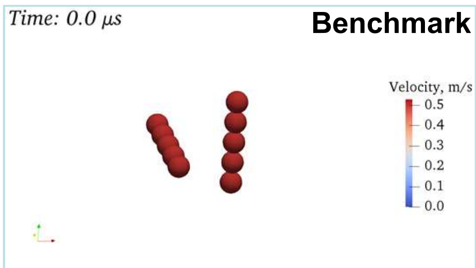
F_cg is the coarse-graining scaling factor

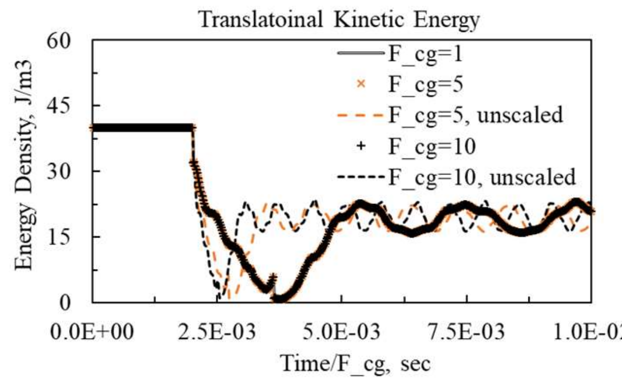
3.3 Performance Evaluation (MS 2.2 & 2.3)

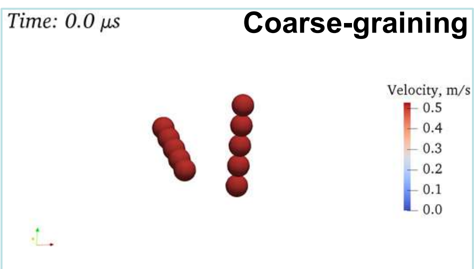
3) Coarse-graining collision & transport

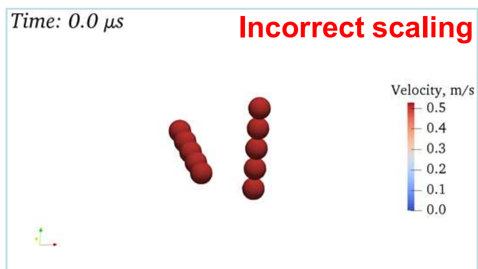
- **Case 2**: switchgrass particle collision
- bonded-sphere + Hertz-Mindlin

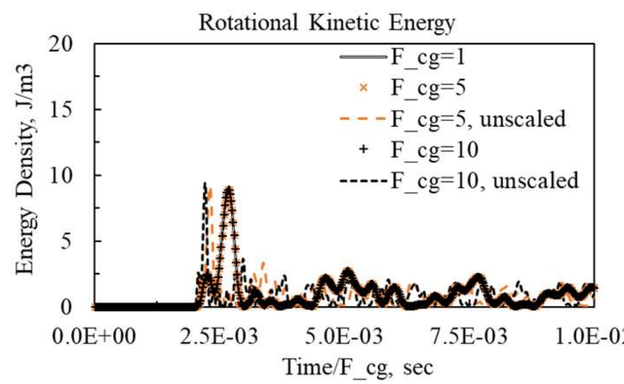












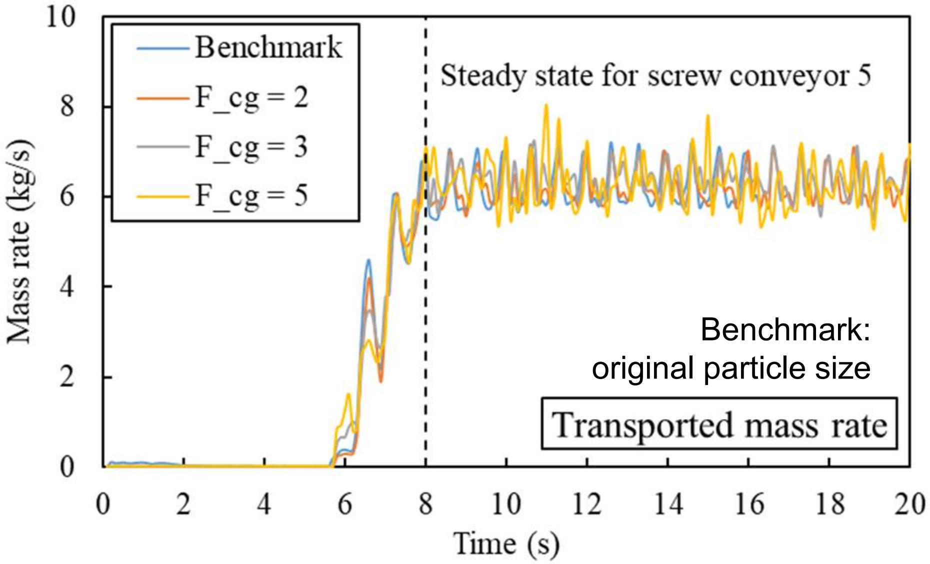
Coarse-graining has <u>< 1%</u> error (total kinetic energy) compared to the benchmark (F_cg=1) both during and after the collision.

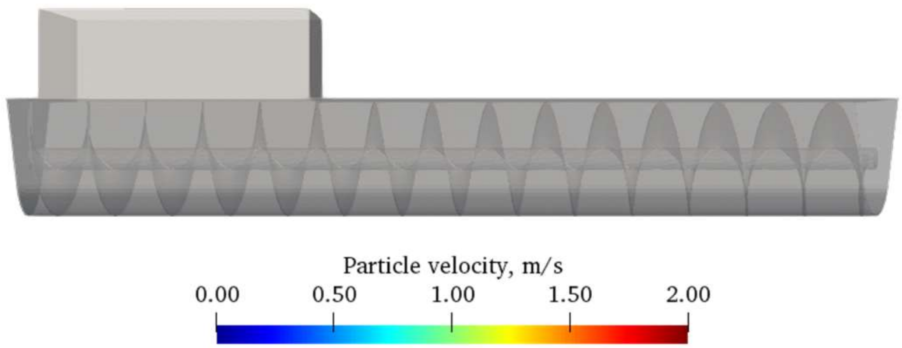
F_cg is the coarse-graining scaling factor

3.3 Performance Evaluation (MS 2.2 & 2.3)

3) Coarse-graining collision & transport

- **Case 3**: screw conveyor-5 transport (10% moisture)
- Liquid bridge + rolling resistance + Hertz-Mindlin

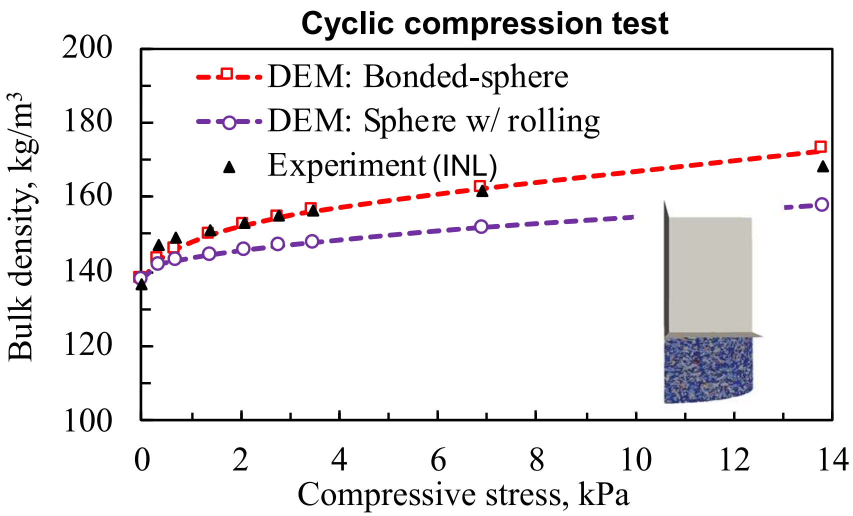


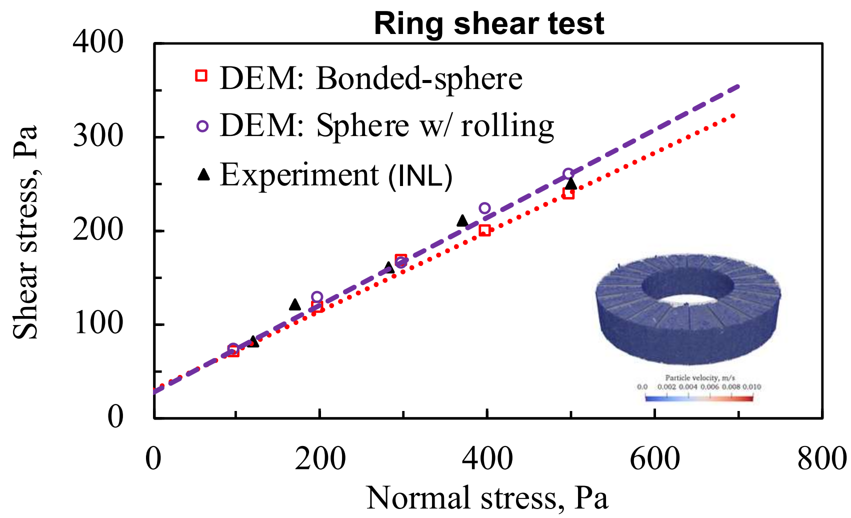


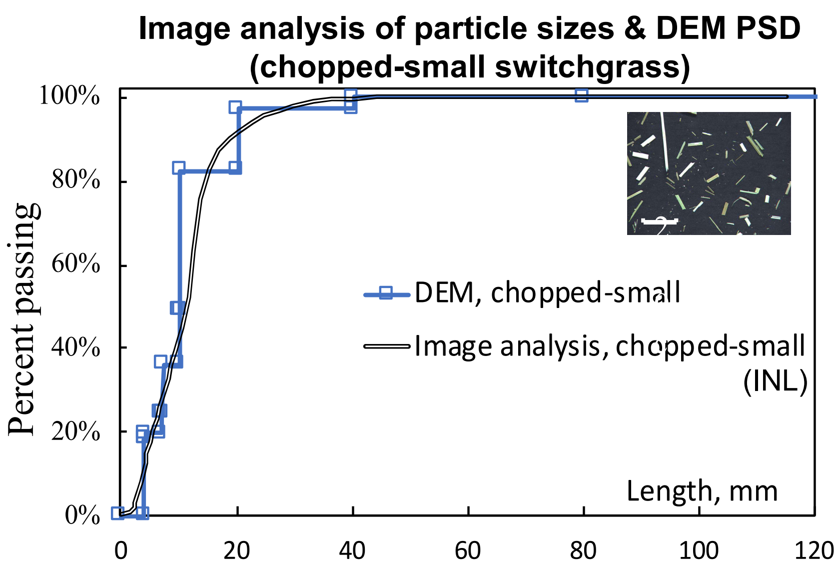
Case	Average transported rate (kg/s)	Error (%)
Benchmark	6.2418	-
F_cg = 2	6.2492	**0.0074**
F_cg = 3	6.3651	**0.1233**
F_cg = 5	6.2956	**0.0538**

3.3 Performance Evaluation (MS 2.2 & 2.3)

4 & 5) Cyclic compression and ring shear tests







Error in compression test

Error, %	Bonded-sphere	Rolling
Average	1.12	4.49
Maximum	2.72	6.17

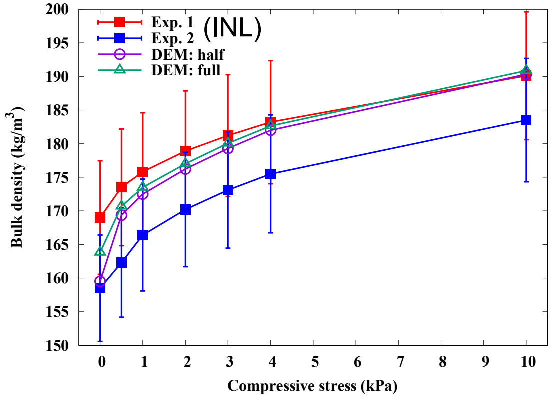
Error in ring shear test

Error, %	Bonded-sphere	Rolling
Average	6.35	4.90
Maximum	13.89	10.62

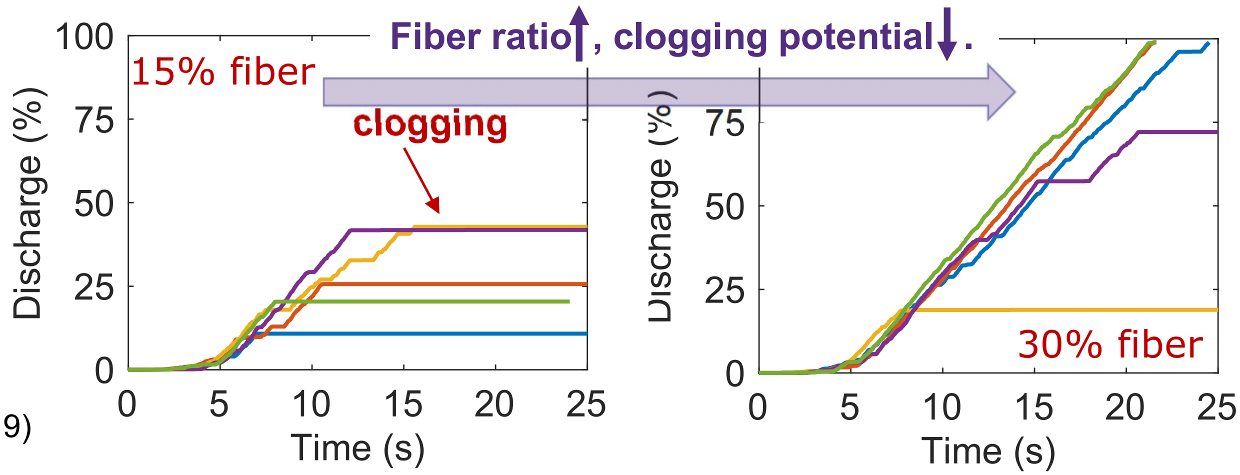
3.3 Performance Evaluation (MS 2.2 & 2.3)

6) Hopper flow tests

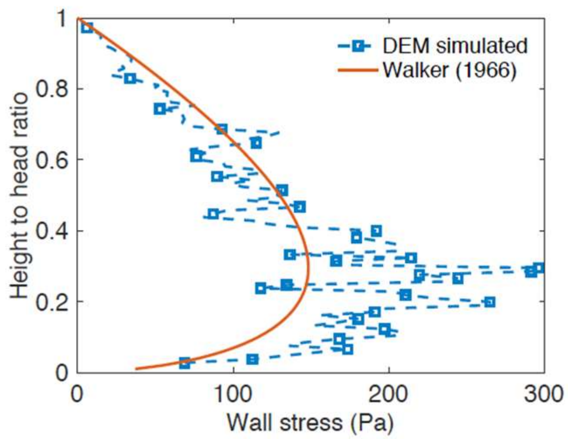
- Parameter calibrated for woodchips (leverage FCIC material handling task)
- Biomass characteristics and flow

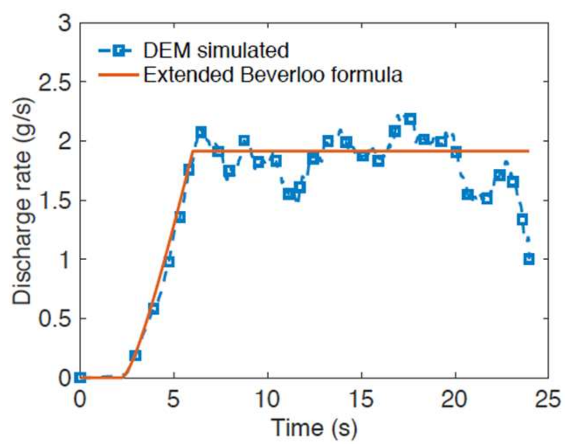


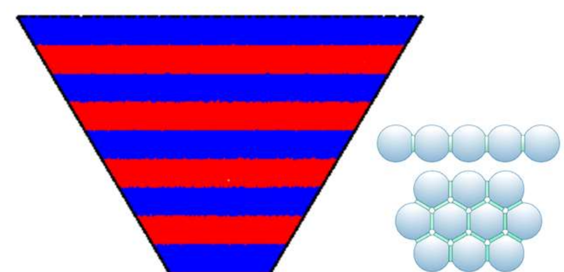
Bulk density vs. stress (Xia et al. 2019)



- Analytical solutions







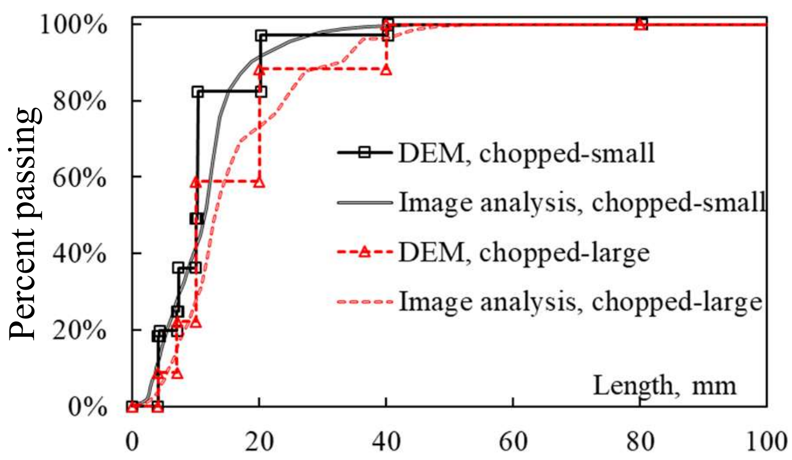
Complex-shaped particles

3.3 Performance Evaluation (MS 2.2 & 2.3)

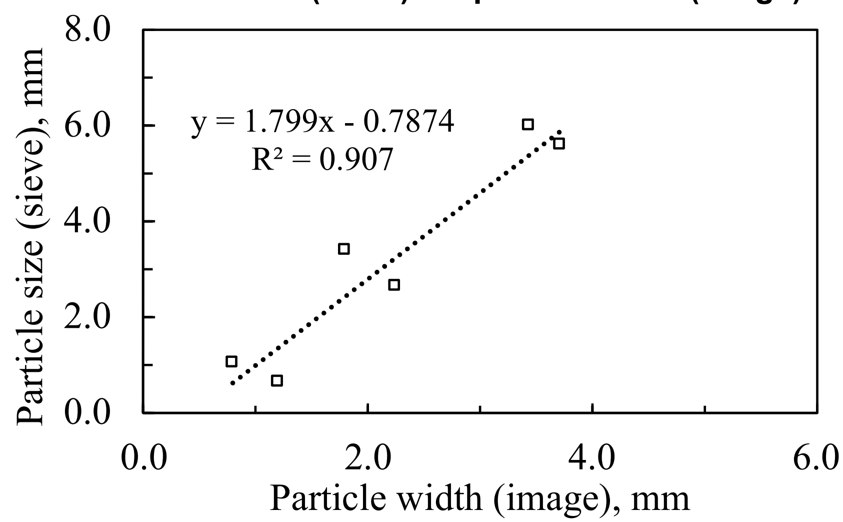
7) Bulk density tests

- Westover et al. 2015 switchgrass data (INL)

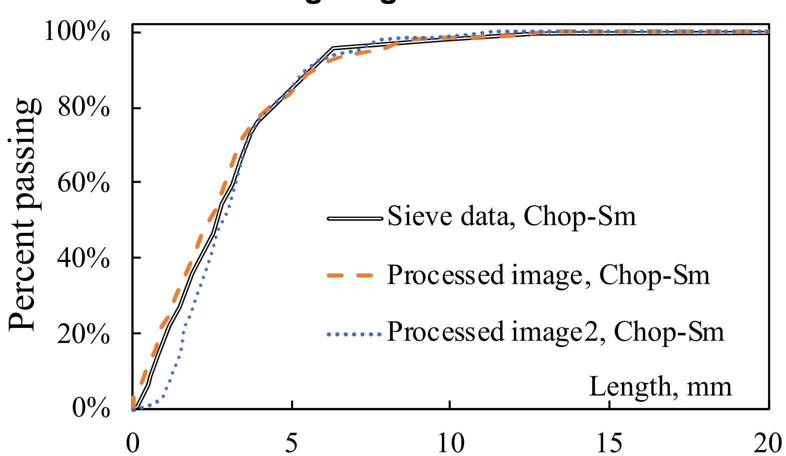
Particle size distribution

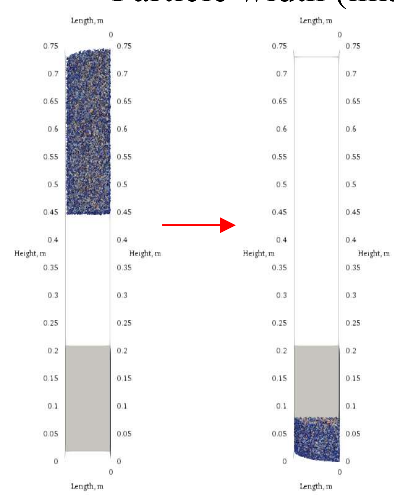


Particle size (sieve) vs. particle width (image)



Predicting length PSD with sieve data

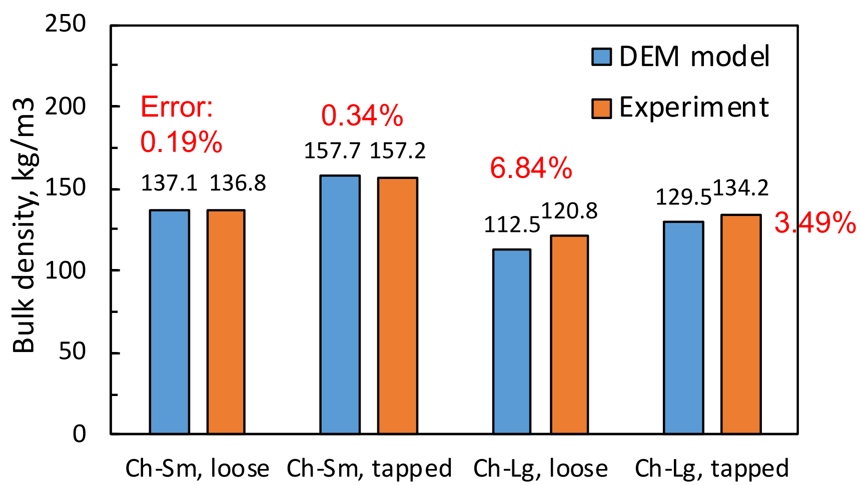


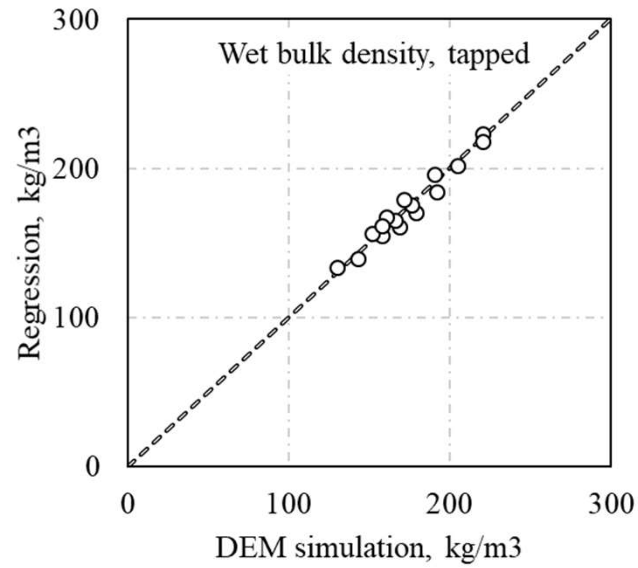


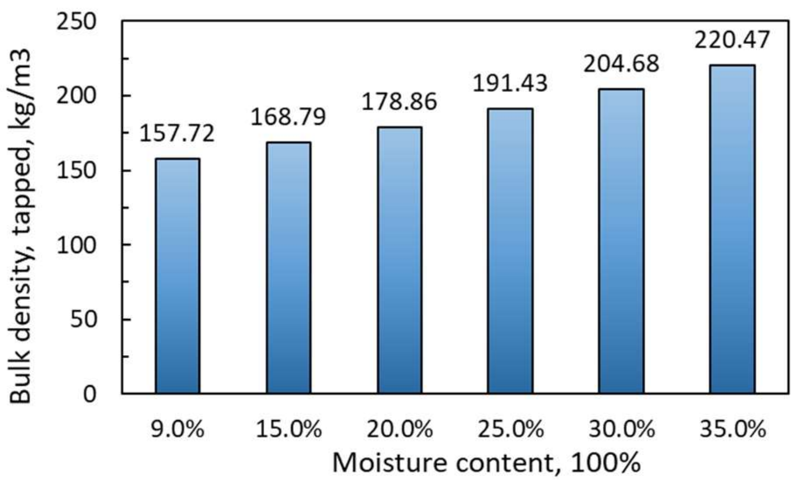
3.3 Performance Evaluation (MS 2.2 & 2.3)

7) Bulk density tests

- Max. error of DEM predicted bulk density is **6.84%**







Dry bulk density, loose:

$$\rho_{d,loose} = 196.4591 - 110.2639 * w + 294.1846 * w^2 - 29.4076 * D_{50} + 1.3616 * {D_{50}}^2 + 0.9191 * D_{90/10} - 0.0700 * {D_{90/10}}^2$$

$$R^2 = 0.9097$$

Wet bulk density, loose:

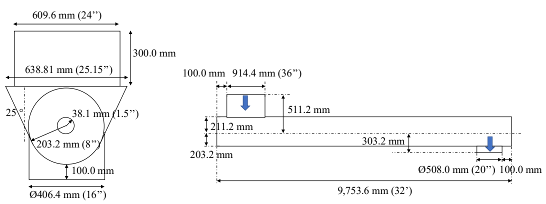
$$\rho_{w,loose} = 220.0079 - 73.3554 * w + 687.6672 * w^2 - 38.5341 * D_{50} + 2.0902 * {D_{50}}^2 + 1.0571 * D_{90/10} - 0.0835 * {D_{90/10}}^2$$

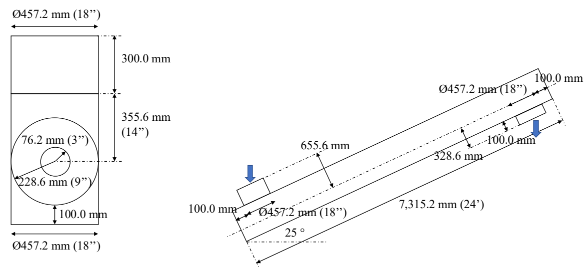
$$R^2 = 0.9573$$

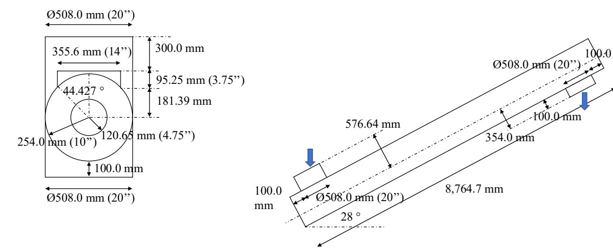
3.3 Performance Evaluation (MS 2.2 & 2.3)

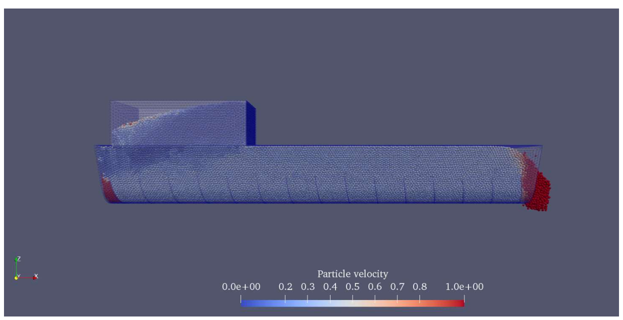
8) Conveyor modeling

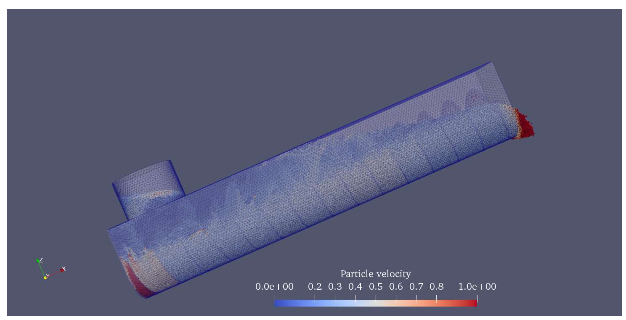
- Screw Conveyor - 1
- Screw Conveyor - 2
- Screw Conveyor - 4

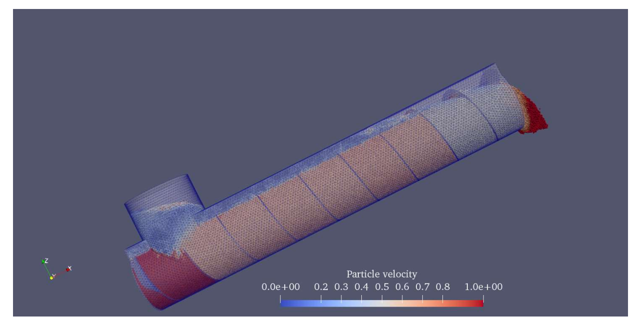










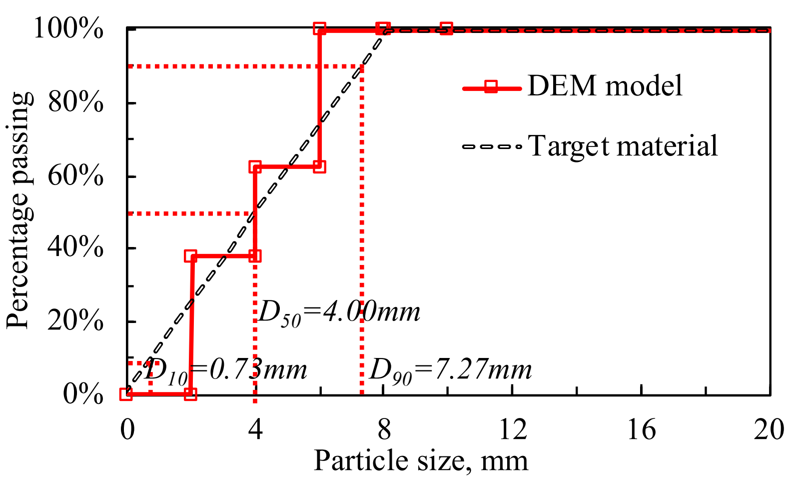


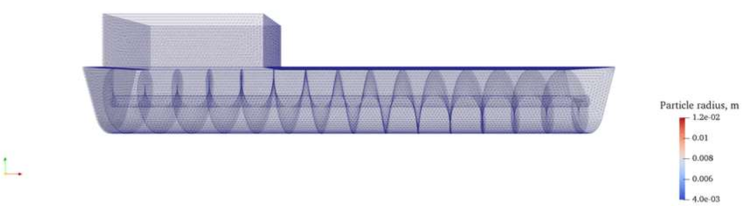
- Dimensions of SC-5 & 6 at PDU are the same as SC-4
- Other PDU units (e.g., drag chain conveyor, hopper, inlet connectors) have been developed

3.3 Performance Evaluation (MS 2.2 & 2.3)

8) Conveyor modeling

- Screw-conveyor-1
- Switchgrass
- Moisture 0-35%
- Various particle size distributions
- Various conveyor speeds





Summary of simulation data (SC-1, partial data shown)

#	D50 mm	D90/D10	Moisture content %	Rotational speed rpm	Contact angle degree	Notes	Biomass stored US ton	Transport rate US ton/h	Average Torque N/m
1	4	10	10	90	75	Baseline	0.0860	24.601	30.089
2	4	5	10	90	75		0.0852	24.304	30.421
3	4	15	10	90	75	D90/D10	0.0861	24.633	30.182
4	3	10	10	90	75		0.0870	25.118	29.247
5	6	10	10	90	75	D50	0.0830	23.559	31.758
6	4	10	0	90	75		0.0860	24.357	30.572
7	4	10	5	90	75		0.0852	24.561	30.739
8	4	10	15	90	75	Moisture	0.0860	24.648	30.386
9	4	10	10	30	75		0.0861	8.688	29.125
10	4	10	10	60	75	Rotation	0.0856	16.337	29.266
11	4	10	10	90	75		N.A.	N.A.	N.A.
12	4	10	10	90	75		0.0875	25.262	29.271
13	4	10	10	90	75		0.0866	24.823	30.104
14	4	10	10	90	75	Scale-up	0.0868	24.956	31.602
15	4	1	10	90	75	D90/D10	0.0848	24.643	28.417
16	4	10	10	45	75		0.0877	13.643	29.772
17	4	10	10	75	75		0.0856	20.426	29.709
18	4	10	10	105	75		0.0868	29.289	31.215
19	4	10	10	120	75	Rotation	0.0875	33.903	31.881
20	4	1	0	90	75		0.0857	24.812	29.501
21	4	1	5	90	75		0.0848	24.643	28.440
22	4	1	15	90	75		0.0849	24.671	28.669
23	4	1	20	90	75		0.0850	24.670	28.821
24	4	1	25	90	75		0.0839	24.680	28.803
25	4	1	30	90	75	Moisture	0.0850	24.691	28.647
26	2	1	10	90	75		0.0858	25.201	27.562
27	3	1	10	90	75		0.0855	24.908	28.062
28	5	1	10	90	75	D50	0.0841	24.356	29.911
29	4	1	5	90	10		0.0840	24.621	27.915
30	4	1	10	90	10		0.0839	24.546	27.419
31	4	1	15	90	10		0.0838	24.526	27.487
32	4	1	20	90	10		0.0838	24.475	27.293
33	4	1	25	90	10		0.0838	24.514	27.235
34	4	1	0	90	10		0.0857	24.766	29.132
35	4	1	30	90	10		0.0838	24.491	27.534
36	4	1	35	90	10	Moisture	0.0837	24.565	27.415
37	2	1	10	90	10		0.0841	24.995	26.308
38	6	1	10	90	10	D50	0.0856	24.740	29.033
39	4	5	10	90	10		0.0849	24.439	29.932
40	4	10	10	90	10		0.0854	24.647	29.979
41	4	15	10	90	10	D90/D10	0.0857	24.779	29.748

Simulation #

Particle size & distribution

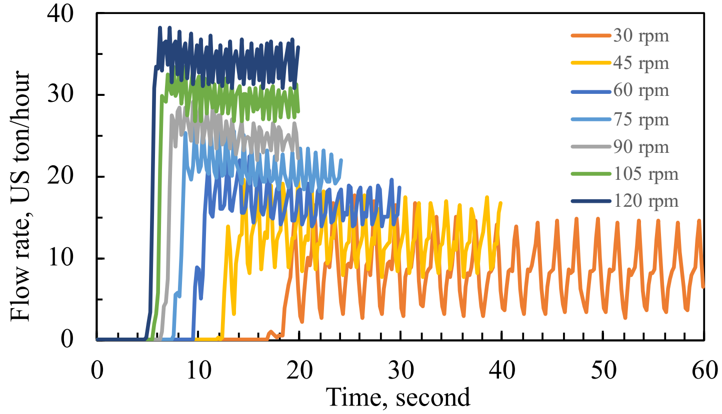
Moisture content

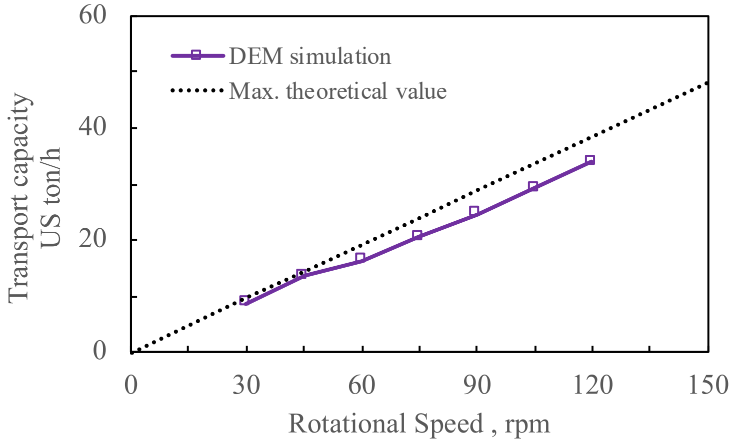
Equipment settings

3.3 Performance Evaluation (MS 2.2 & 2.3)

8) Conveyor modeling

- Evaluated against a theoretical model for maximum transport

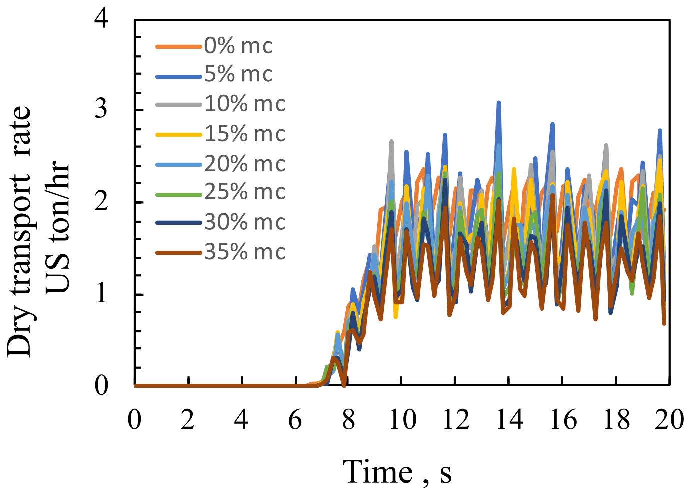


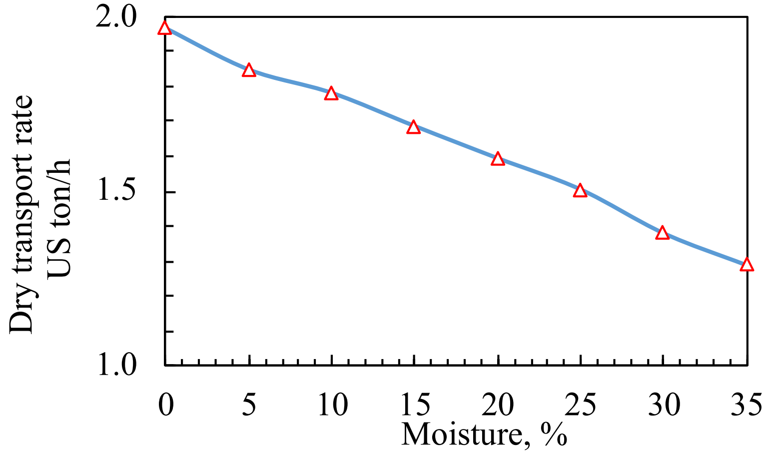


Average error:
12.08%

Max. error:
15.03%

- Moisture 0 – 35% at PDU operating transport range (2 US ton/h)





Valid. w/ new PDU data

3.3 Performance Evaluation (MS 2.2 & 2.3)

No.	Test name	Evaluation	DEM Results
1	Bending & axial loading	Analytical	**~1%** error
2	Collision of moisture particles	Analytical	**~1%** error
3	Coarse-graining collision & conveyor transport	Energy density	**~1%** error for particle collision; **~ 2%** for conveyor transport
4	Cyclic compression	Experiments	Ave **~1.12%** (bonded-sphere) Ave **~4.49%** (rolling)
5	Ring shear	Experiments	Ave **~6.35%** (bonded-sphere) Ave **~4.90%** (rolling)
6	Hopper flow	Experiments / empirical	Within experimental bond
7	Bulk density	Experiments	Ave **~2.71%**; Max **~6.84%**
8	Conveyor modeling	Experiments / analytical	Ave **~12.08%**; Max **~15.03%**

Go/No-Go

- DEM has been extensively evaluated with analytical, empirical, and experimental results/data at the particle, lab, and PDU-scales.
- DEM yields satisfactory results (most cases <10% error) for capturing biomass characteristics (particle size distribution, moisture) and modeling their impacts on material/system responses (strength, bulk density, flow).
- *Meet the Go criteria for DEM model performance.*

OUTLINE

1. Project Overview

2. Milestones and Go/No-Go

Go/No-Go Criteria

3. Performance of DEM models

4. Usefulness and Quality of INL Data

4.1 Historical switchgrass and corn stover data

4.2 New PDU experiments

5. Ongoing and Future Work

6. Summary

4.1 Historical Data (Lab)

Historical switchgrass data from INL

(Westover et al., 2015)

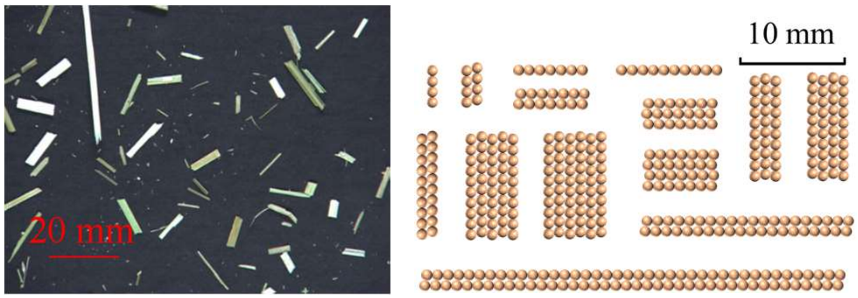
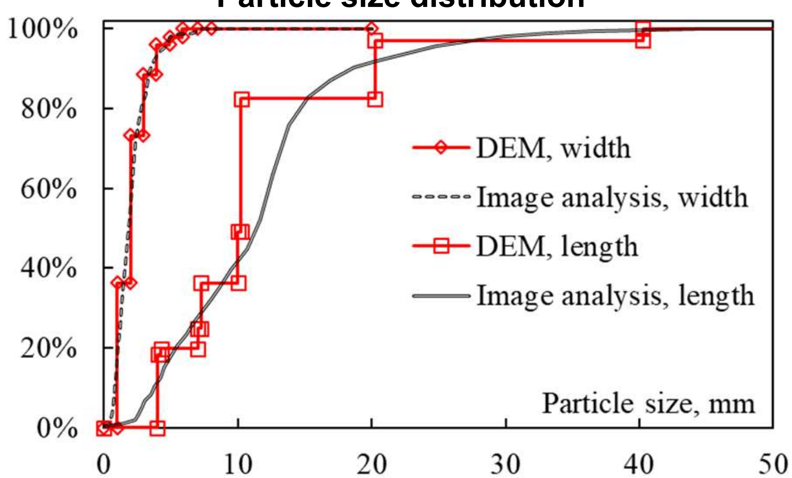


Image analysis and DEM shape templates

Particle size distribution



Biomass characteristics table

	Grind-Lg	Chop-Lg	Grind-Sm	Chop-Sm
W50, mm	2.68	1.81	2.09	2.26
W10, mm	1.19	0.80	1.03	1.21
W90, mm	5.19	3.46	3.74	3.72
L50, mm	46.4	13.4	11.4	11.5
L10, mm	11.7	5.6	3.8	3.8
L90, mm	104.0	32.7	33.4	19.1
Bulk density-loose, kg/m3	72.2	92.9	120.8	136.8
Bulk density-tapped, kg/m3	90.2	108.0	134.2	157.2
Frictional angle, deg.	27.5	29.3	28.8	23.8
Cohesion, Pa	101.9	56.1	79.5	37.2

Compression test data

Compressive	Bulk density, kg/m3			
stress, kPa	Grind-Lg	Chop-Lg	Grind-Sm	Chop-Sm
0.34	89.6	103.1	127.0	146.8
0.69	93.1	107.4	129.3	148.7
1.37	97.7	113.0	132.4	151.2
2.06	101.1	116.9	134.6	153.1
2.76	103.8	119.1	136.6	154.6
3.44	106.1	121.5	138.5	156.0
6.90	115.1	131.0	145.7	161.7
13.80	126.4	147.8	156.0	168.0
34.50	149.1	172.4	175.0	183.0
68.90	173.9	198.7	196.9	199.9
139.00	207.3	235.1	228.9	224.3
345.00	275.2	310.3	296.2	274.7

Westover, T., Phanphanich, M., and Ryan, J. 2015. Comprehensive rheological characterization of chopped and ground switchgrass. Biofuels, 6(5-6): 249-260.

4.1 Historical Data (PDU)

Data available

1. Density for corn stover:

   - Bale density: Moisture level:
     - Low (5.5%,)
     - Medium (16.8%)
     - High (24.2%)

Bulk density values of the bale (kg/m³)

Moisture Level	Average Density (kg/m^3)
Low	138.60
Medium	107.00
High	105.20

- Density after grinder 1 and grinder 2 under the following settings:
  - In-feed rate: 2%, 5%, 10%, 20%, 30% of the full capacity.
  - Grinder mill speed: 36 Hz, 41 Hz, 51 Hz, 60 Hz
  - Moisture level:
    - Low (G1=10.4%, G2=19.1%)
    - Medium (21.7%, 19.1%)
    - High (30.3%, 30.9%)

Bulk density values after G1 and G2 (kg/m³)

Grinder Speed (in Hz)	Moisture Level					
	Grinder 1			Grinder 2		
	Low	Medium	High	Low	Medium	High
36	30.64	34.39	35.39	72.43	71.22	63.59
41	35.67	34.90	32.01	77.19	66.58	62.94
51	36.95	31.19	36.86	75.95	62.48	58.50
60	37.93	40.67	36.80	77.42	69.05	61.60

4.1 Historical Data (PDU)

2. Particle size distribution for corn stover:

- After grinder 1 and grinder 2:
  - In-feed rate: 2%, 5%, 10%, 20%, 30% of the full capacity.
  - Grinder mill speed: 36 Hz, 41 Hz, 51 Hz, 60 Hz
  - Moisture level: Low, medium and high
  - Screen size: Grinder 1: 1”, 2”, 3”, 4”, 6”; Grinder 2: 1”

3. Particle size distribution for switchgrass :

- After grinder 1 and grinder 2:
  - Moisture level: Low, medium and high

Missing data:

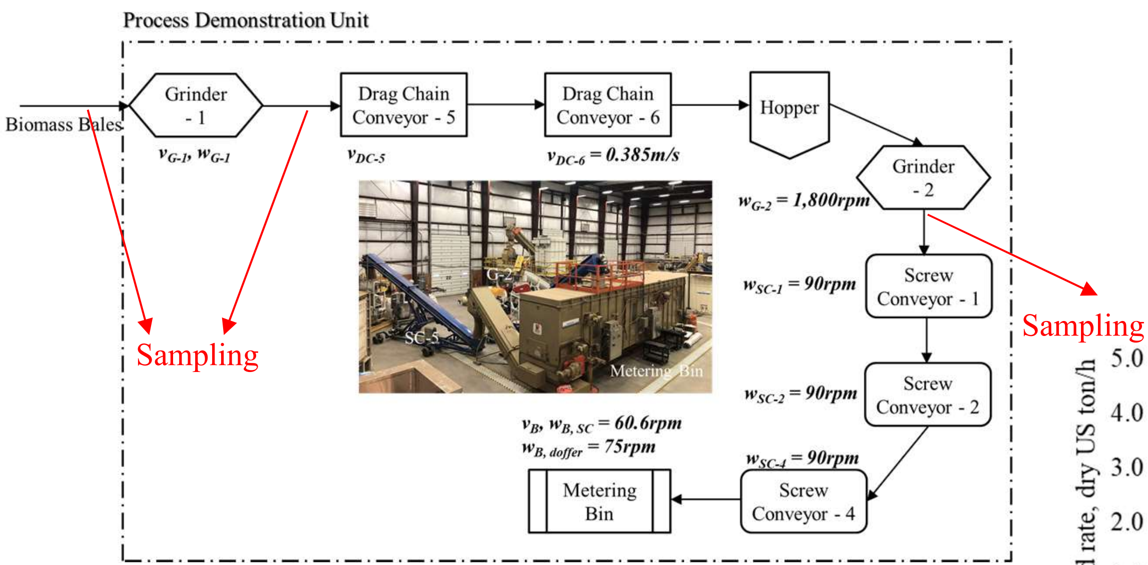
- Density and moisture of switchgrass
- Mechanical data for corn stover
- Density and particle size distribution for miscanthus
- Machine failure
- Energy consumption based on particle size distribution, moisture level

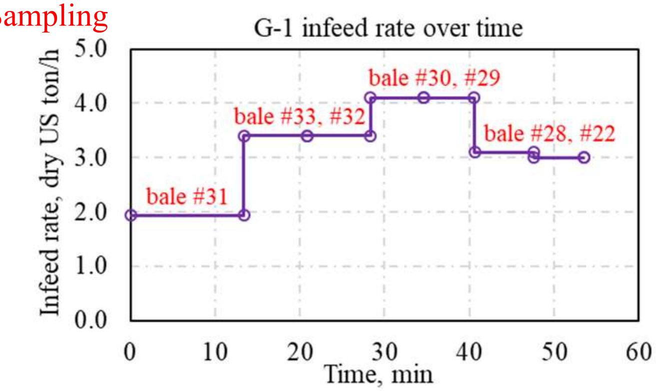
4.2 New Data (PDU)

PDU test 1

- Objective: to provide additional data (switchgrass) for PDU unit scale model development and validation
- Material: switchgrass (7 bales in total, 5 in dry & 2 in wet)
- Data: July 17, 2019

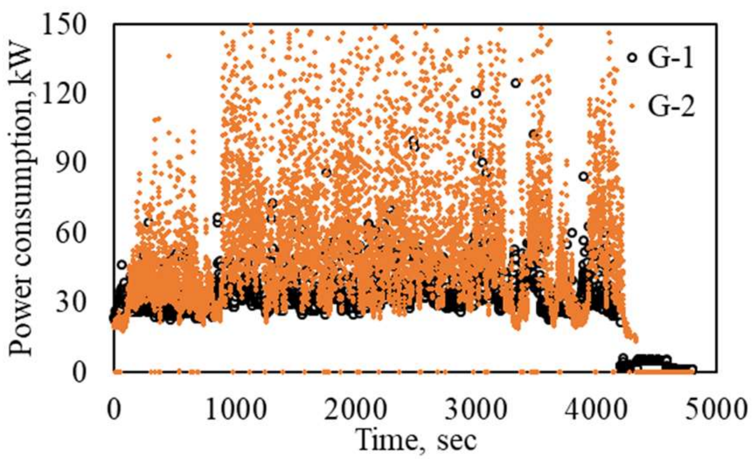
1) Test setup

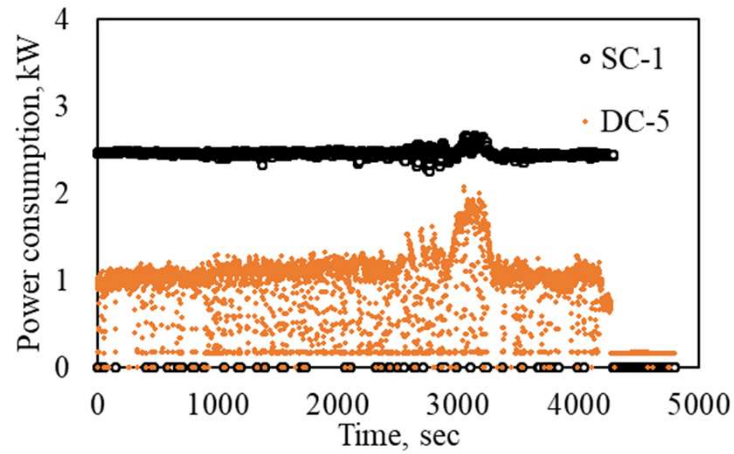




4.2 New Data (PDU)

2) Power consumption data





3) Preliminary switchgrass characteristic data

	Moisture content, %		Loose bulk density, kg/m3		Tapped bulk density, kg/m3		D50, mm		D10, mm		D90, mm		D90/D10
	Mean value	STD	Mean value	STD	Mean value	STD	Mean value	STD	Mean value	STD	Mean value	STD	
Bale#31, bale	12.1	N.A.	N.A.	N.A.	N.A.	N.A.	6.50	N.A.	1.86	N.A.	32.23	N.A.	17.34
Bale#33, bale	13.6	N.A.	N.A.	N.A.	N.A.	N.A.	8.33	N.A.	1.94	N.A.	30.89	N.A.	15.91
Bale#32, bale	13.6	N.A.	N.A.	N.A.	N.A.	N.A.	8.46	N.A.	1.85	N.A.	29.08	N.A.	15.76
Bale#30, bale	11.8	N.A.	N.A.	N.A.	N.A.	N.A.	7.16	N.A.	1.78	N.A.	29.94	N.A.	16.80
Bale#29, bale	12.6	N.A.	N.A.	N.A.	N.A.	N.A.	8.84	N.A.	2.12	N.A.	30.60	N.A.	14.44
Bale#28, bale	25.0	N.A.	N.A.	N.A.	N.A.	N.A.	7.13	N.A.	1.82	N.A.	28.58	N.A.	15.71
Bale#22, bale	25.0	N.A.	N.A.	N.A.	N.A.	N.A.	19.77	N.A.	2.60	N.A.	41.75	N.A.	16.08
Bale#31, after G-1	12.53	1.28	39.13	1.98	54.37	2.11	2.13	0.100	0.52	0.039	6.24	0.193	11.95
Bale#33, after G-1	11.83	1.32	39.16	3.19	56.10	3.68	1.94	0.135	0.47	0.032	5.90	0.355	12.68
Bale#32, after G-1	12.19	0.96	39.86	1.00	56.68	0.23	2.21	0.017	0.56	0.011	7.15	0.889	12.86
Bale#30, after G-1	11.38	0.74	48.00	4.17	65.81	3.97	1.97	0.072	0.48	0.020	5.66	0.529	11.90
Bale#29, after G-1	11.26	0.37	47.05	4.38	61.85	1.80	2.10	0.049	0.52	0.019	5.75	0.246	11.09
Bale#28, after G-1	19.53	1.53	41.20	4.40	53.91	6.69	2.31	0.010	0.59	0.009	7.23	0.097	12.15
Bale#22, after G-1	27.7	5.00	52.87	3.11	86.39	22.58	1.77	0.406	0.45	0.073	4.61	0.950	10.24
Bale#31, after G-2	11.52	1.27					0.68	0.042	0.24	0.019	1.48	0.024	6.27
Bale#33, after G-2	10.96	1.47					0.63	0.088	0.24	0.063	1.42	0.086	6.01
Bale#32, after G-2	11.33	1.03					0.66	0.045	0.23	0.021	1.47	0.029	6.34
Bale#30, after G-2	11.35	0.50					0.67	0.041	0.23	0.016	1.47	0.035	6.45
Bale#29, after G-2	10.02	1.21					0.71	0.090	0.23	0.025	1.48	0.039	6.49
Bale#28, after G-2	16.39	0.63					0.73	0.018	0.24	0.003	1.49	0.006	6.17
Bale#22, after G-2	22.86	1.46					0.61	0.038	0.17	0.020	1.49	0.024	8.61

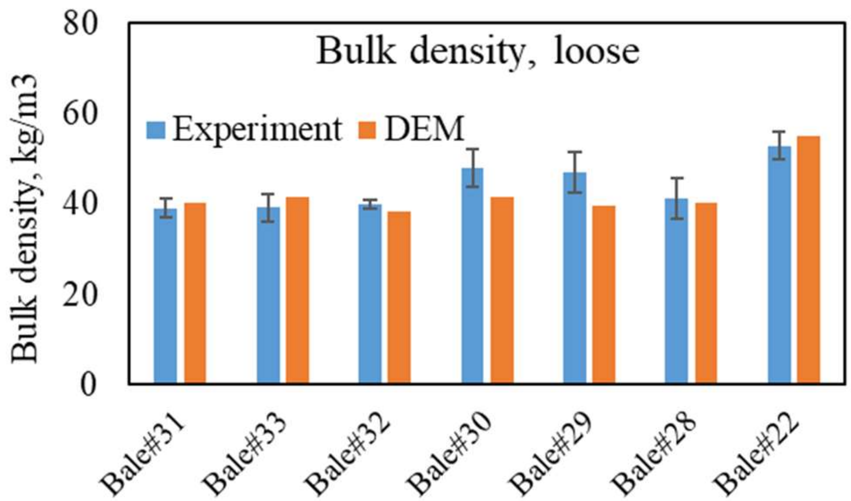
On average, a very small (1.71%) moisture change before and after G-2.

4.2 New Data (PDU)

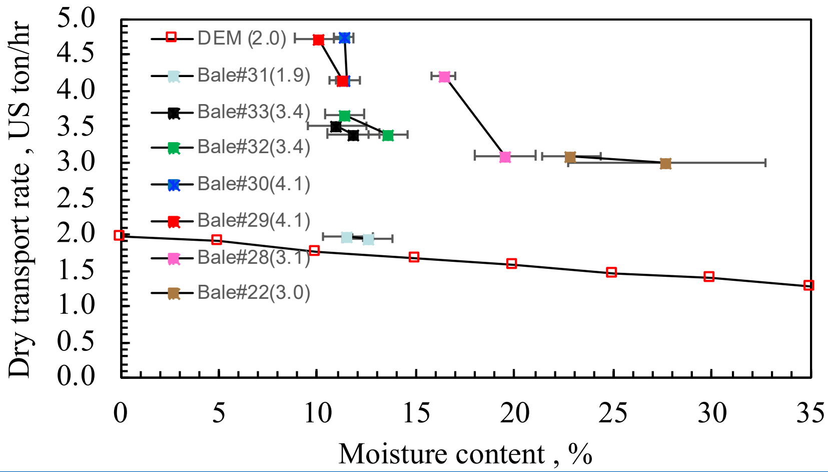
4) Preliminary DEM validation results

- **Bulk density**

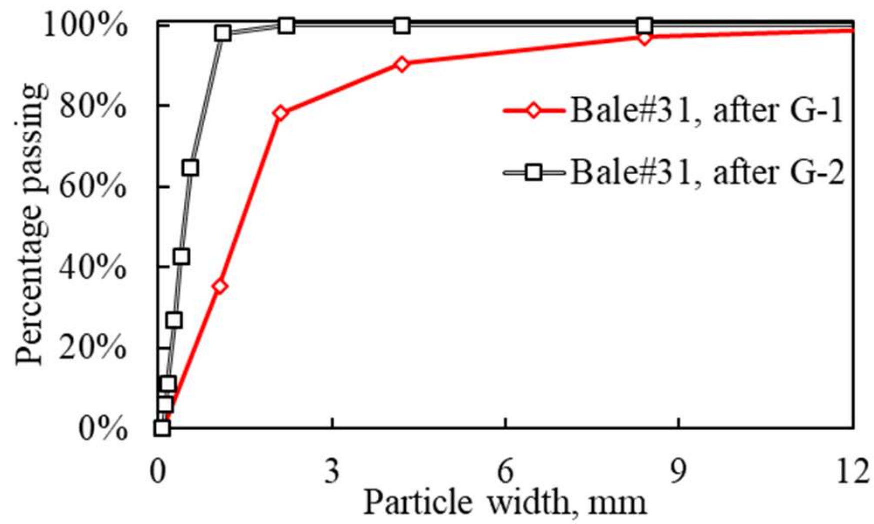
- Error: 6.91% (average); 15.81% (max)

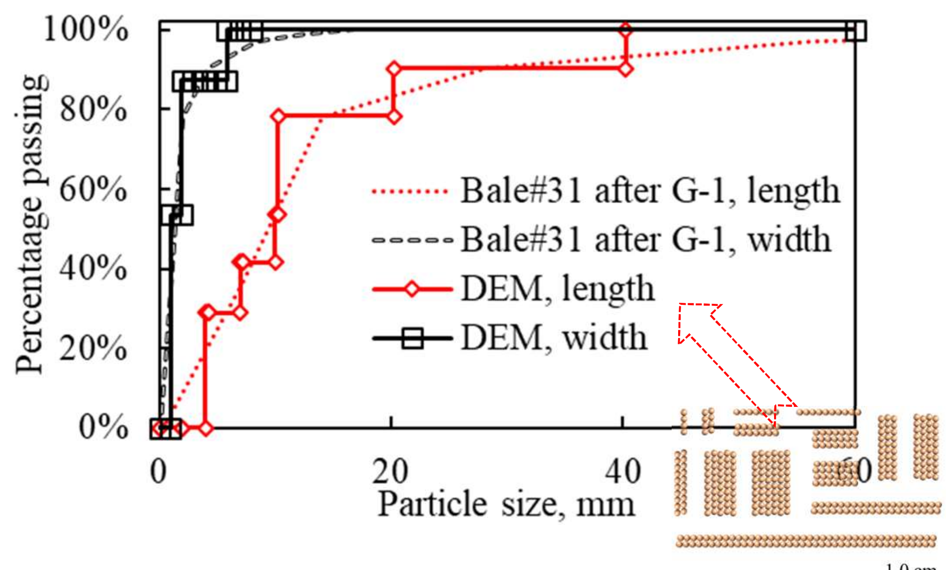


- **Flow data**



- **Particle size distribution:**





DEM particle templates

4. Usefulness and Quality of INL Data

Go/No-Go:

- Historical INL data (both lab and PDU data) are useful and of quality for our DEM and mathematical model development.
- There are limitations in historical data; some key data are missing.
- Additional PDU experiments are performed (7/17) and planned to generated data for further DEM and mathematical model development.
- *Meet the Go criteria for data.*

OUTLINE

1. Project Overview

2. Milestones and Go/No-Go

Go/No-Go Criteria

✓ 3. Performance of DEM models

✓ 4. Usefulness and Quality of INL Data

5. Ongoing and Future Work

6. Summary

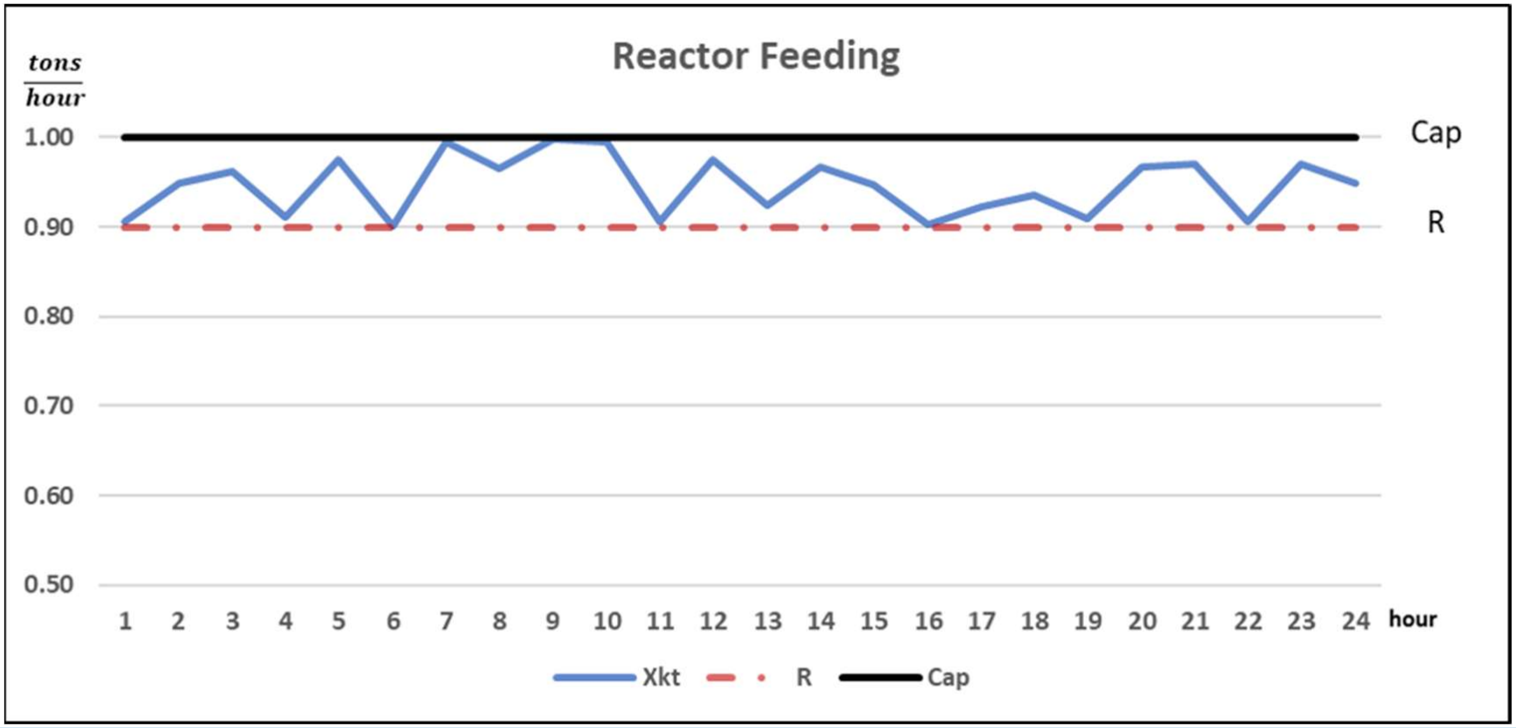
5. Ongoing and Future Work

Year 2: System Optimization model:

Objective:

1. Maintain a continuous flow of biomass to the reactor by identifying values for the control variables.
2. Ensure that reactor's utilization is at least 90%.

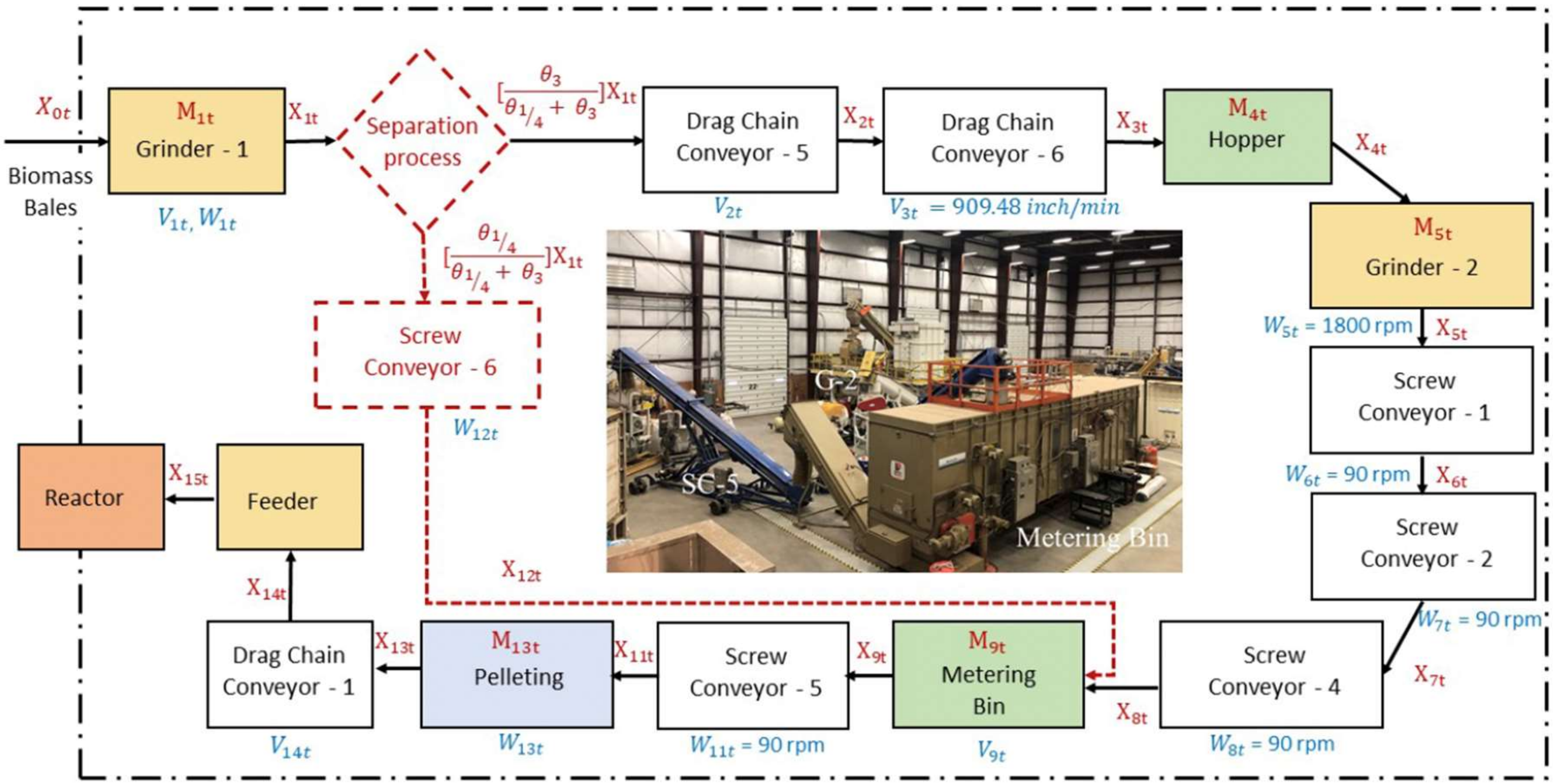
Control variables: In-feed rate, rotational speed of the conveyors, rotational speed of grinding equipment, and inventory level.



5. Ongoing and Future Work

Approaches used:

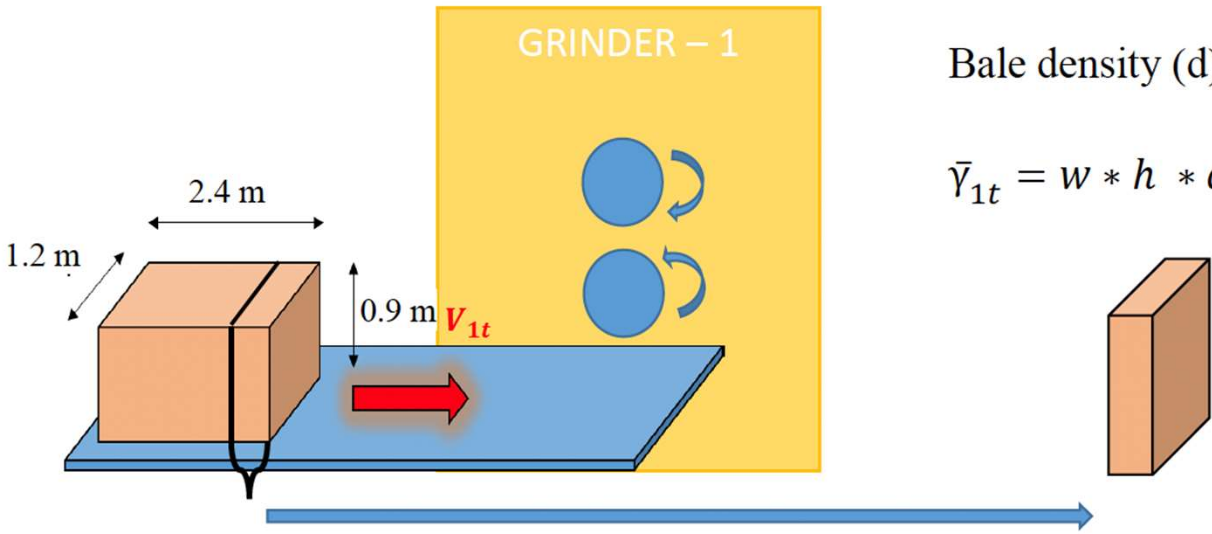
- Deterministic models: Inventory control, Network flow, System reliability
- Stochastic models: Queuing, Chance constraint optimization, 2-stage stochastic programming



5. Ongoing and Future Work

Integrating DEM with mathematical models:

1. Biomass density impacts flow into an equipment.



Bale density (d) = 0.209 tons/m³

$$\bar{\gamma}_{1t} = w * h * d = 1.219 * 0.914 * 0.209 = 0.233 \text{ tons/m}$$

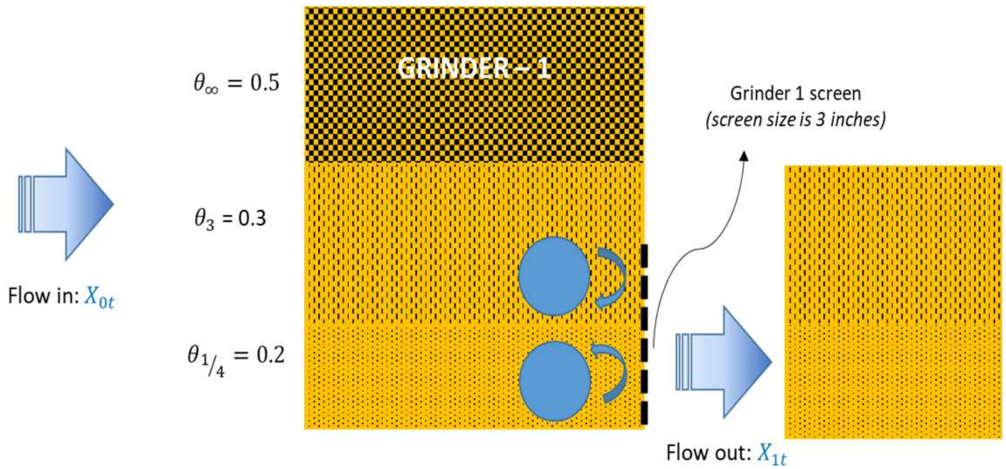
X_{0t} the amount of biomass fed to the system in period t

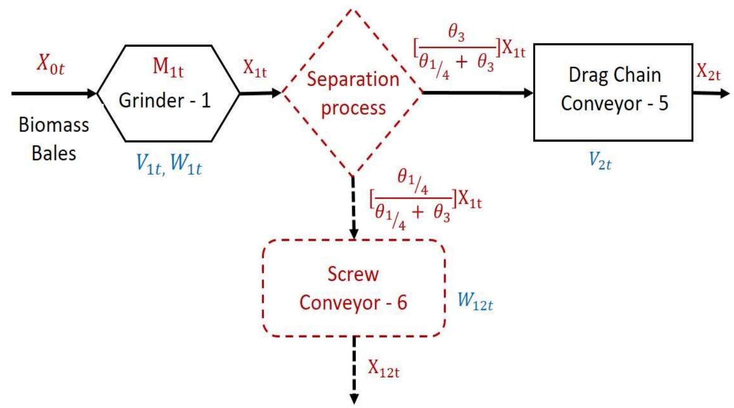
$$X_{0t}\ (\text{tons/min}) \quad \leq \quad \tilde{\gamma}_1\ (\text{tons/m})\ V_{1t}\ (\text{m/min}) \quad \forall t \in T.$$

5. Ongoing and Future Work

Integrating DEM with mathematical models:

2. Biomass particle size impacts the flow from the separation process.





3. Particle size distribution $(D_{50}, \frac{D_{90}}{D_{10}})$ and moisture (m) impact density, thus, impact the flow in the system:

$$Density = c + \alpha_1 m + \alpha_2 m^2 + \alpha_3 D_{50} + \alpha_4 D_{50}^2 + \alpha_5 \frac{D_{90}}{D_{10}} + \alpha_6 \left(\frac{D_{90}}{D_{10}}\right)^2$$

Values of coefficients *c* and *α* are gathered from DEM results.

4. Machine failure: time between failures for given biomass characteristics, time to repair.

5. Ongoing and Future Work

Year 3:

1. Testing at INL's PDU

    Planned Feedstocks: Corn stover, Switchgrass, Miscanthus

    Feedstock standard: Moisture 10%-30%; Ash 5%-15%

    QA/QC process: Inspect each bale to measure moisture and ash contents

2. Integrate the analytical models into a could-based Decision Support System (DSS).

    Create an alpha version of a cloud-based DSS.

    Provide an opportunity to store data, run computations, and visualize results.

This task is supported by UTSA's Open Cloud Institute and UTSA's Simulation, Visualization and Real Time Prediction Center.

6. Summary

Year 1 effort: Develop and validate 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).

Go/No-Go

✓ **I. DEM performance evaluation**

- DEM extensively evaluated with analytical, empirical, and experimental results/data at the particle, lab, and PDU-scales.
- DEM yields satisfactory results (most cases <10% error) for capturing biomass characteristics (particle size distribution, moisture) and modeling their impacts on material/system responses (strength, bulk density, flow).

✓ **II. Historical and new INL data** are useful and of quality for the proposed model development and validation

✓ **III. Ongoing and future work:** PDU tests for DEM validation, optimization model development, and future PDU demonstration.

6. Summary

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). (Task 2.2)
- Z. Lai, Y. Xia, H. Huang, T. Westover, L.K. Jordan, and Q. Chen, "Investigation and characterization of the particle deformability effects on granular hopper flow based on DEM simulations", in review, (2019). (Task 2.2 & 2.3)

Presentations

- Y. Guo, Q. Chen, Y. Xia, M. Roni and S. Eksioglu, "Discrete element modeling of chopped switchgrass: particle size and shape effects on bulk mechanical properties", The 2019 Engineering Mechanics Institute and Geo-Institute Specialty Conference, Pasadena, CA, (2019). (Task 2.2 & 2.3)
- Y. Xia, Z. Lai, Q. Chen, T. Westover, J. Klinger and H. Huang, "Discrete element modeling of granular flow of flexible woody biomass particles", The 2019 Engineering Mechanics Institute and Geo-Institute Specialty Conference, Pasadena, CA, (2019). (Task 2.2 & 2.3)
- B. Gulcan, S.D. Eksioglu, M. Roni, K. Castillo, "Integrated Process Optimization for Biochemical Conversion," Presentation at the IISE Annual Meeting, Orlando, FL (2019). (Task 4.1)
- 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). (Task 2.2)

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