DOE Bioenergy Technologies Office (BETO)

Analytical Modeling of
Biomass Transport and Feeding Systems
EE0008256
WBS 3.1.1.005 (previously WBS 3.5.3.4)

Updated
Feb 19 2021

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Jim Dooley, Dale Monceaux,
John Aston, Marcial Gonzalez, Kingsly Ambrose, Klein Ileleji,

Collaborators: INL, ANL, Forest Concepts, AdvanceBio, Penn State

Project Overview

Project goals are:

- Develop strong and innovative computational models that rigorously represent flow performance of biomass materials.
- Verify models in cooperation with the Idaho National Laboratory using INL pilot scale equipment.
- Support technology development and engineering solutions that economically and sustainably overcome critical barriers associated with handling of solids in biorefinery production process.

1 – Management

Michael Ladisch
Project Director

DOE
Mark Shmorhun
Jessica Phillips

Carl Wassgren,
David Thompson, Nathan Mosier
Pankaj Sharma
Project Co-Directors

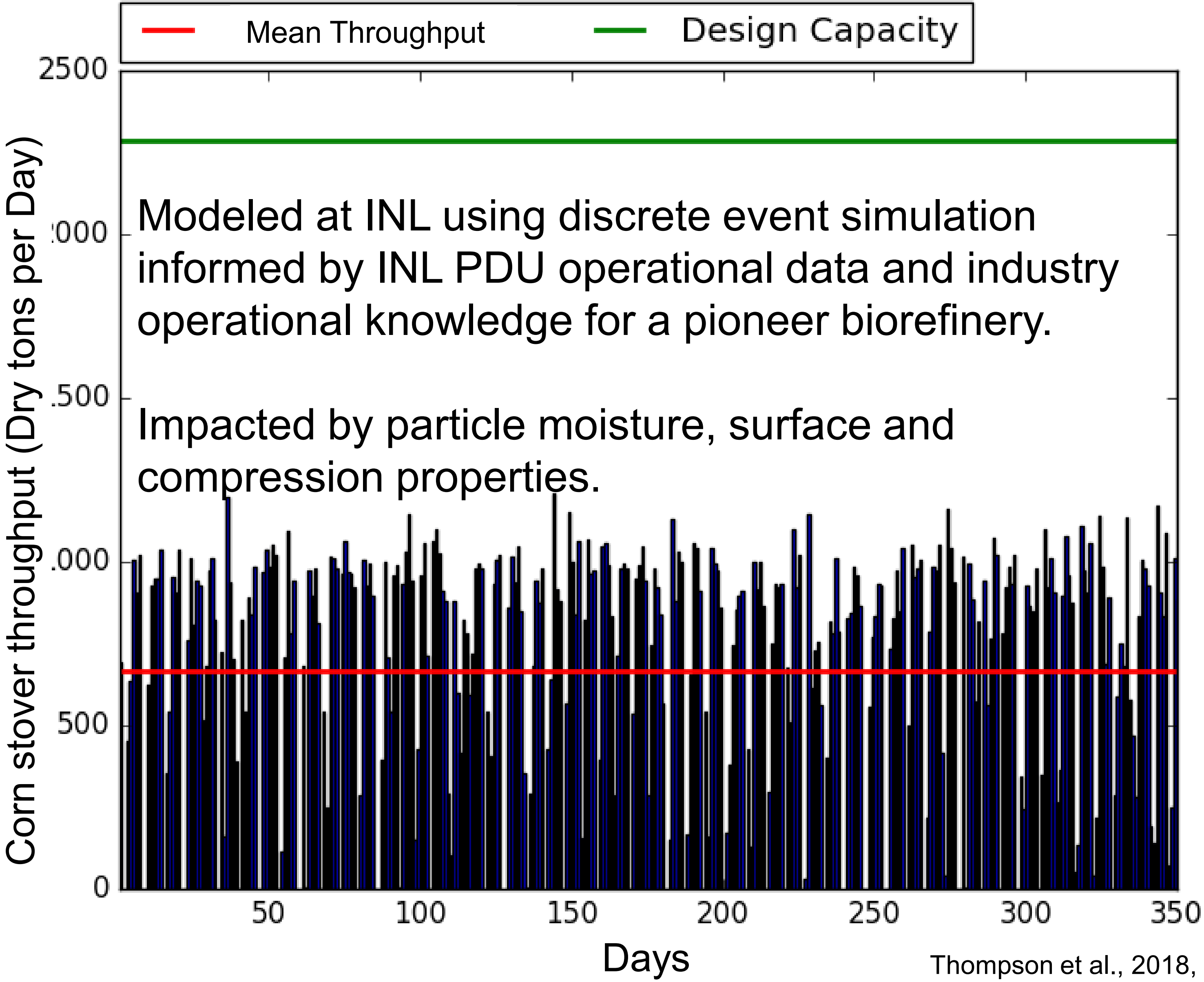
Modeling	Characterization	Verification	LCA / TEA
Carl Wassgren, Lead Marcial Gonzalez Arezoo Ardekani	Eduardo Ximenes, Lead Kingsley Ambrose Kendra Erk Klein Ileleji	David Thompson, Lead John Aston Jim Dooley Dale Monceaux	Nathan Mosier, Lead Abigail Engelberth Pahola Thathiana Benavides Gallego

Monthly management meetings (Purdue, INL, ANL, Forest Concepts, AdvBio, DOE) review results, next steps, schedule. Research teams meet biweekly In addition, investigators meet weekly with students and colleagues.

2 – Approach

- Develop accurate, innovative computational and empirical models that rigorously represent the multiphase flow of biomass materials.
- Modeling to be based on knowledge of the impact of the effect of moisture, temperature, and pressure on feedstock handling.
- Characterization of physical, structural, and compositional properties of biomass feedstocks will be compared to results from computational models using actual flow behavior of biomass materials in a biorefinery.
- Verify the new analytical models at INL and determine LCA for the feeding section of a biorefinery with ANL at the completion of modeling.
- A combination of discrete element method (DEM) and finite element method (FEM) modeling is being used.
  - New contact force model implemented in DEM to account for high pressures
  - Continuum FEM model using Drucker Prager Cap (DPC) has not been previously applied to screw feeders

3 - Economic Impact



Modeled at INL using discrete event simulation informed by INL PDU operational data and industry operational knowledge for a pioneer biorefinery.

Impacted by particle moisture, surface and compression properties.

Thompson et al., 2018, 2020

3 – Overall Impact

Impact if successful:

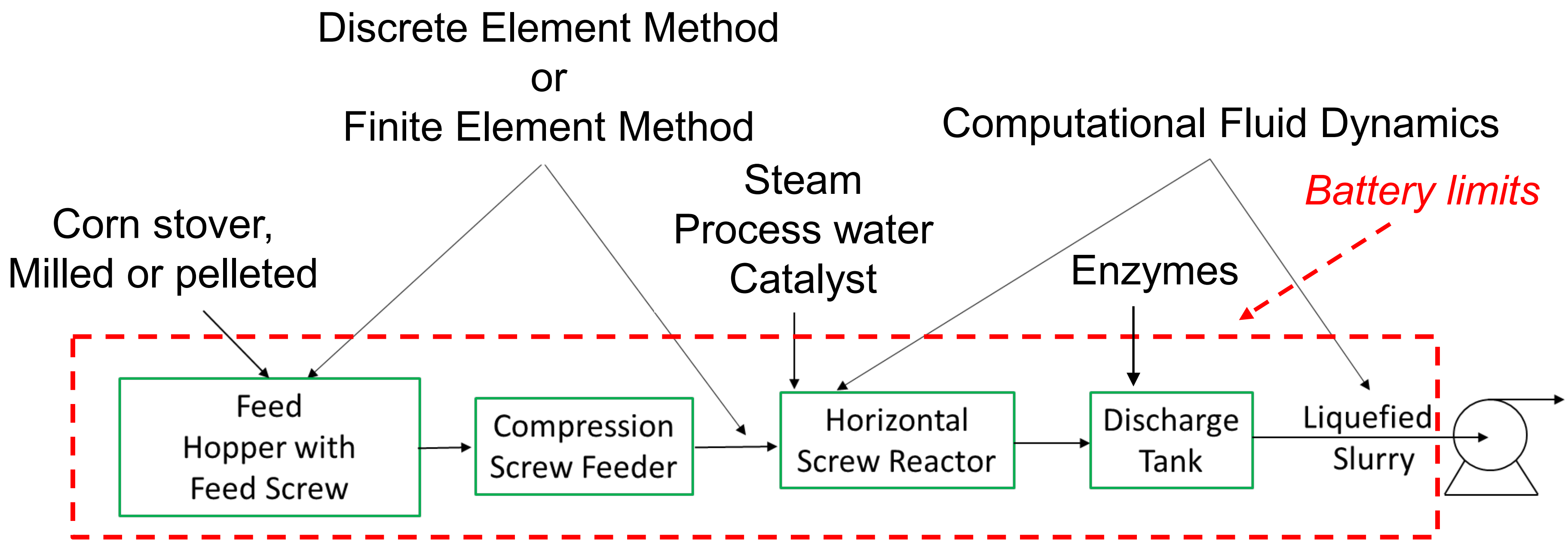
- Increase utilization rate of biorefinery
- Improves efficiency of use of capital
- Approach design capacity through de-bottle-necking
- Possible reduction in operational expenses
  - Enzyme costs
  - Higher productivity

Industry engagement

- Stake-holders meeting with industrial contacts

4 – Progress and Accomplishments

Process Operations Block Diagram Schematic

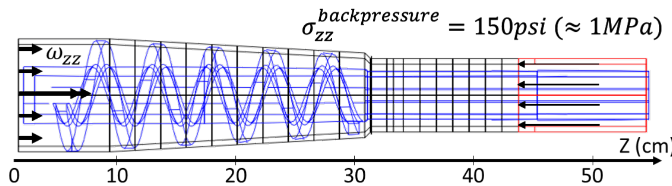


Feedstock, material and energy input → GREET → GHG emissions, FFC consumption, Water consumption

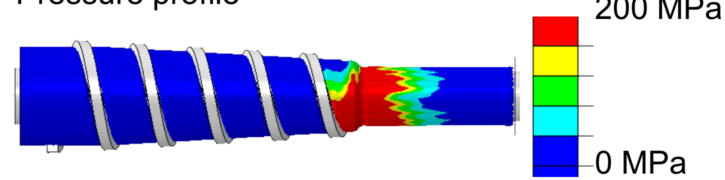
4 – Progress and Accomplishments
Task 1 Summary - Modeling

Task	Technical Accomplishments
1.1 DEM modeling	• Compression screw model setup measurement methods setup complete • Calibration setup complete **Go/No-Go Decision Pt 1 (Dec 1. 2018, 9 months from start of project):** Software installed and operational and demonstrated with preliminary model of pellets (complete)
1.2 FEM modeling	• Partial calibration of model at different moisture contents • Preliminary results generated using assumed material properties **Go/No-Go Decision Pt 2 (April 1, 2019, 13 months from start):** FEM software operational, demonstrated preliminary model with ground corn stover feeding (complete)
1.3 CFD modeling	**Milestone 1.1.3 (Feb 1, 2019, 11 months from start) :** CFD code modified to model slurries, demonstrated preliminary results for rheology (complete)

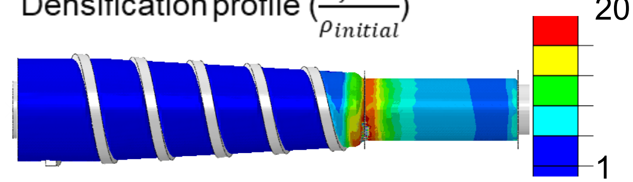
Green = completed

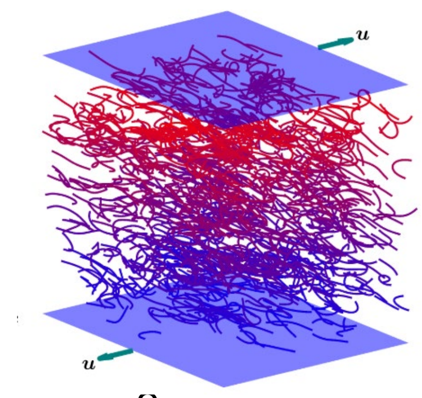


Pressure profile



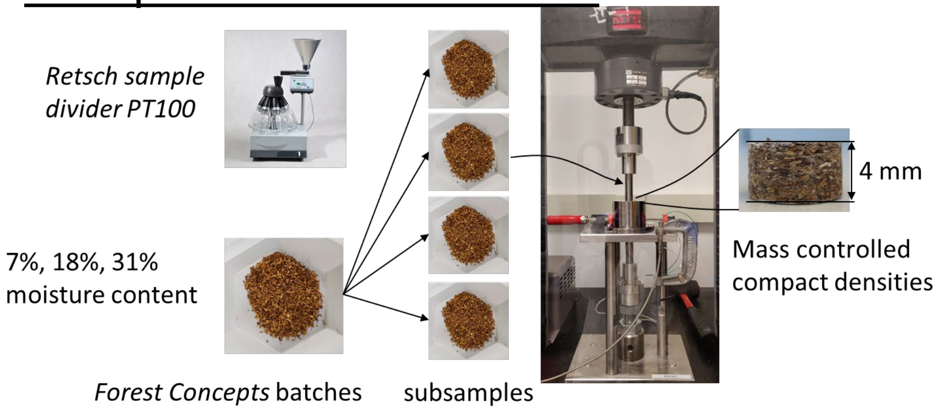
Densification profile $(\frac{\rho_{final}}{\rho_{initial}})$



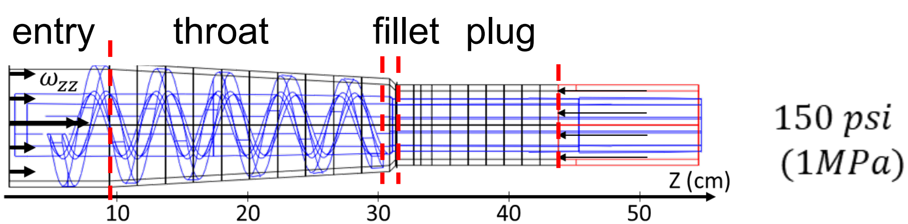


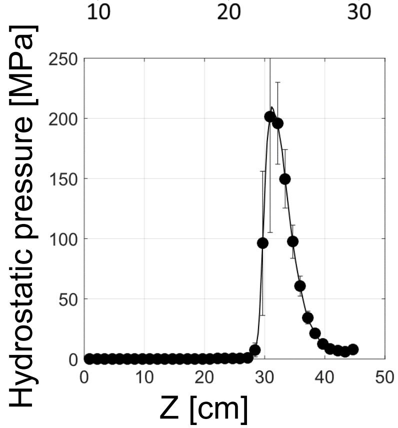
4 – Progress and Accomplishments
Task 1.2 – FEM modeling results

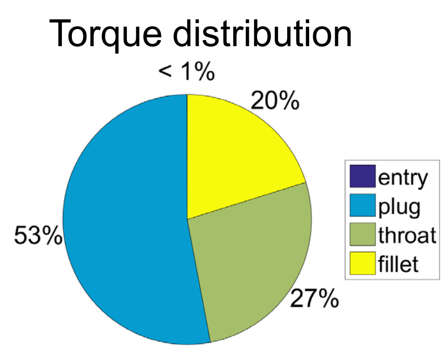
1. Experimental Calibration



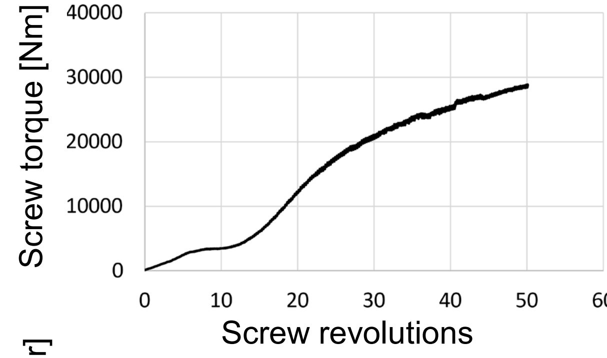
2. Optimized FEM model

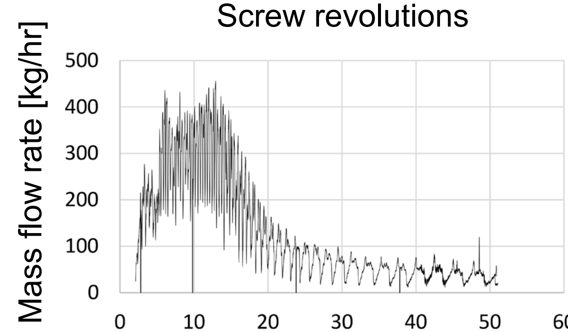


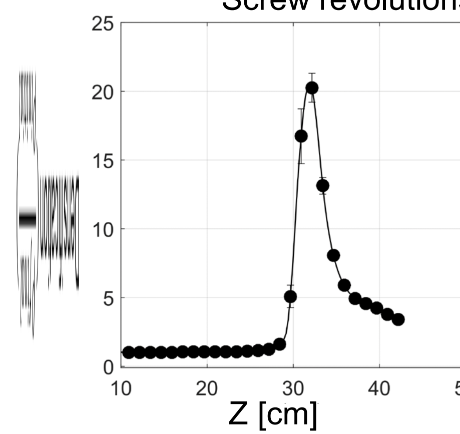




3. Output parameters



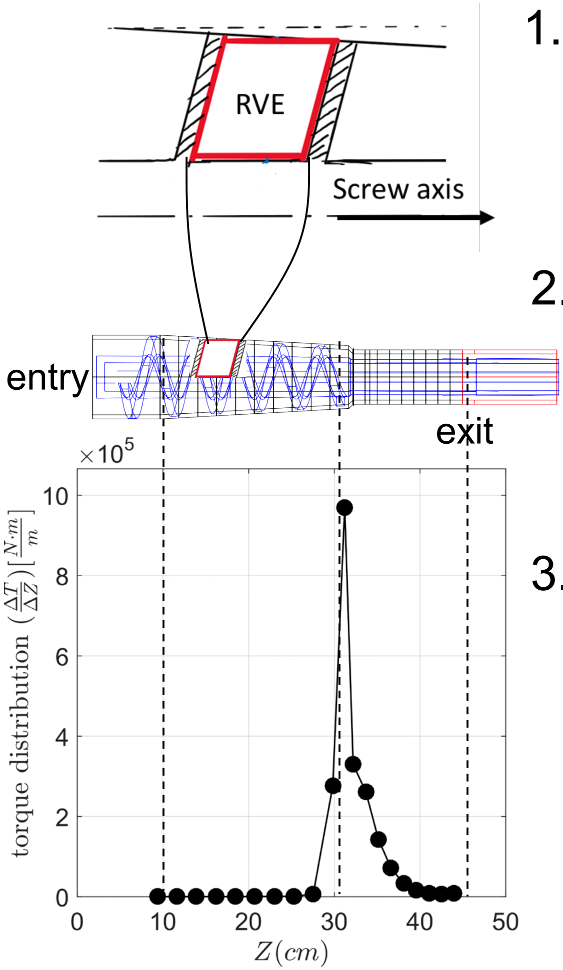




4 – Progress and Accomplishments

Task 1.2 - modeling

Approach:-

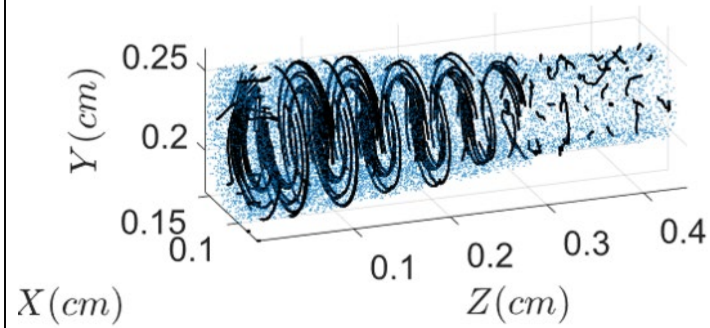


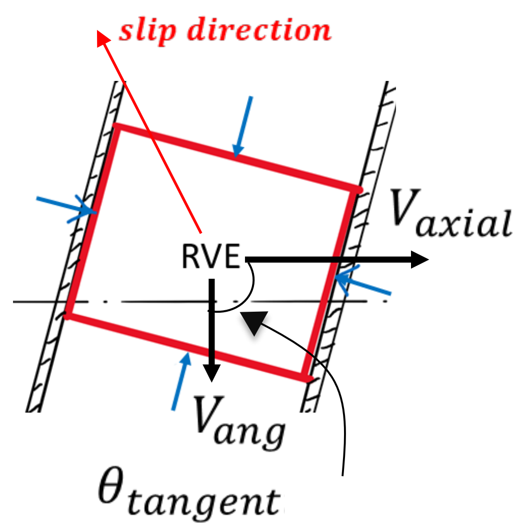
1. **Kinematic analysis**
   FEM results are used to study dynamics of flow in the feed screw

2. **Reduced calibration**
   Die compaction for calibrating hardening properties and wall friction properties

3. **Torque calculation**
   Analytical equation validated by the FEM model will calculate screw torque, mass flow rate and plug density

Step 1: Kinematic analysis

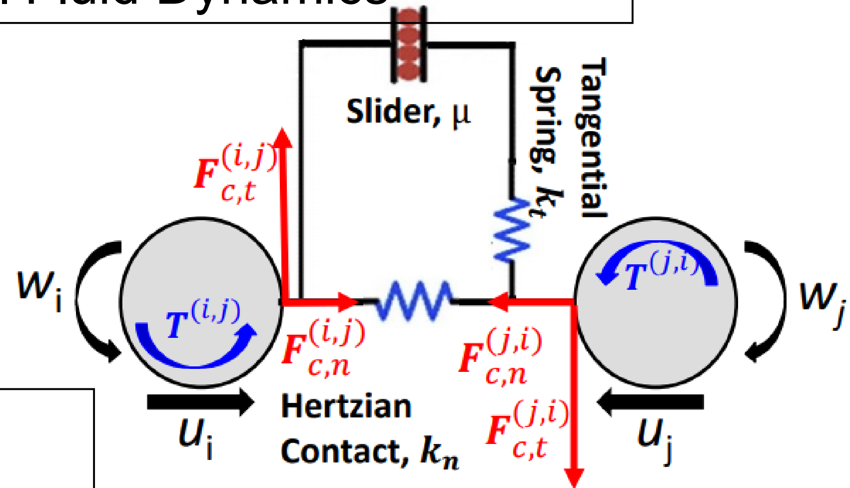




4 – Progress and Accomplishments

Task 1.3 – Computational Fluid Dynamics

Computational approach to modeling the dynamics of particles in a solvent.



Determine the forces and torques acting on each particle in the system. (weight, contact forces, cohesive forces, fluid forces)

↓

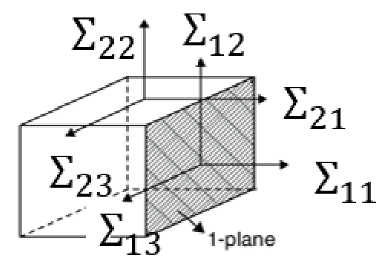
Newton's 2nd Law to determine each particle's acceleration. (translational and rotational)

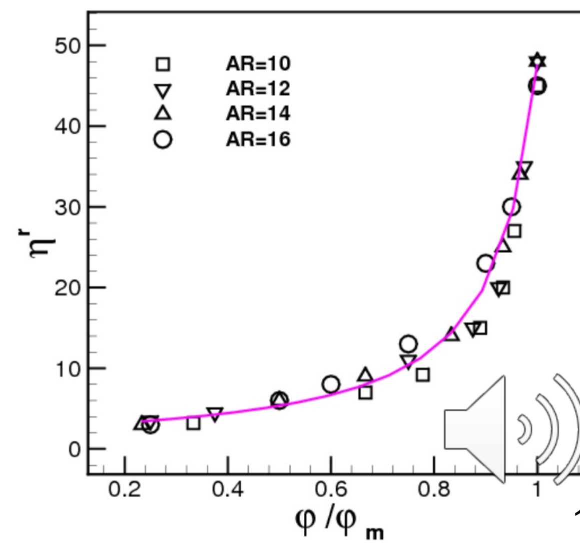
↓

Integrate accelerations in time to find the new particle states. (velocity, position, rotational velocity, orientation)

↓

Calculate variables of interest (stresses, viscosity, yield stress, etc.)





4 – Progress and Accomplishments

Tasks 2.0, 2.1, 2.2 - Compositional and Physical Analysis

Task	Description	Status / Technical Accomplishments
2.0	Corn stover procurement	**Milestone 2 (Mar 1, 2018; prior to project start):** 10 dry ton bales to INL, 10 dry ton bales to Forest Concepts.
2.1	Corn stover milling, pelleting, stabilization and supply	**Milestone 2.1.1 (Mar 1, 2018; 4 months from project start):** 10 kg rotary sheared delivered to Purdue. **Milestone 2.1.2 (Mar 1, 2018; 4 months from project start):** 10 kg pellets delivered to Purdue. Storage in dry, stable conditions: indoors in supersacks
2.2	Corn stover standardization	**Milestone 1.1.3 (Feb 1, 2019, 11 months from start; 6, 18, 30 months from project start):** Standardization completed at INL; corn stover feed plug delivered to Purdue for analysis.




Green = completed.

4 – Progress and Accomplishments

Task 2.2: Selection of Corn Stover Format

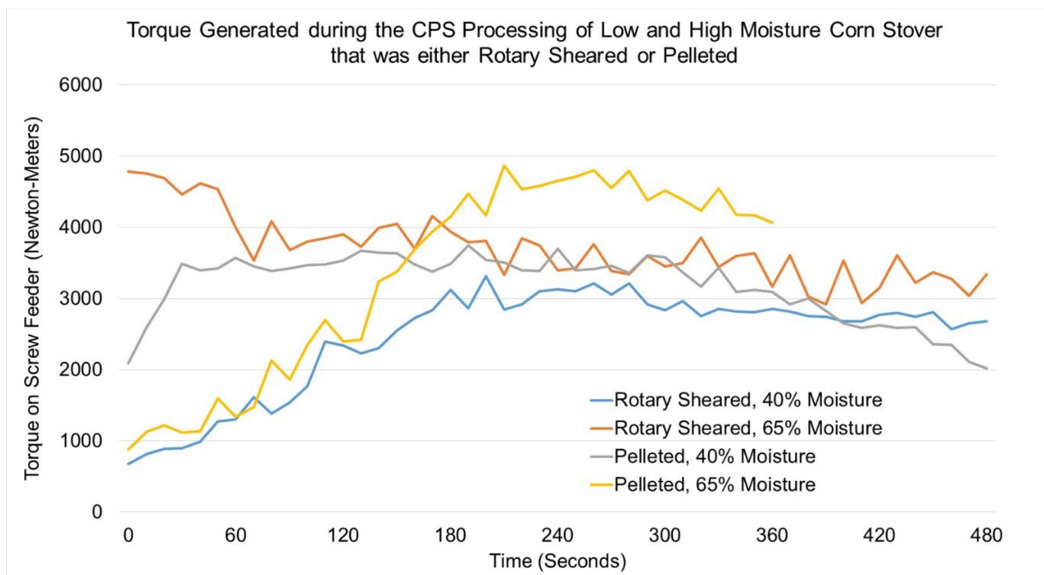
2.2	Selection of corn stover format for model verification testing New Since BP1 Review	**INL Q3 Milestone (June 30, 2020)** At least 10 kg (dry weight) of maleic acid liquified material will be produced from aggregates (plug material) formed using the CPS compression screw feeder from one of two formats: (1) Rotary sheared particulates described in the Corn Stover Procurement, Formatting and Supply Task; or (2) Corn stover pellets described in the Corn Stover Procurement, Formatting and Supply Task The format that is liquefied using maleic acid will depend on the outcome of the maleic acid lab testing with aggregates (plug material) individually prepared from the two formats. Liquefaction will be carried out in the CPS batch reactors at pressure specifications provided by **Purdue (< 200 psig).**

Green = completed. Brown = in progress.

4 – Progress and Accomplishments

Task 2.3, 2.4: Plug Flow Testing

Task	Description	Status / Technical Accomplishments
2.3	Plug flow testing	**Milestone 2.3.1 (Dec 1, 2018; 9 months from project start):** Formation of plug with rotary sheared stover **Milestone 2.3.2 (Dec 1, 2018; 9 months from project start):** Formation of plug with pellets Materials at 40% and 65% moisture content
2.4	Verification of plug integrity in pressurized reactor	**Milestone 3.2 (18 and 21 mon from start)** with rotary sheared and pelleted corn stover **Milestone 2.4.2:** with pelleted stover



Green = completed
Brown = in progress
Red = not completed

4 – Progress and Accomplishments

Task 2.5 – Production of Corn Stover Plug Material

Task	Description	Status / Technical Accomplishments
2.5	Production of 10 kg of plug material in reactor pressurized to at least 150 psig from both rotary sheared and pelleted corn stover. New since BP1 Review	**INL Q1 FY20 Milestone (12/31/19):** Production of Corn Stover Plug Material in Pressurized Reactor **Completed**
3.1	Batch CPS Maleic Acid Liquefaction of Corn Stover Pellets Produced in the Corn Stover Procurement, Formatting and Supply Task New Since BP1 Review	**INL Q2 Milestone (March 31, 2020):** At least 10 kg (dry weight) of maleic acid liquified material will be produced from the corn stover pellets described in the Corn Stover Procurement, Formatting and Supply Task. Liquefaction will be carried out in the CPS batch reactors at pressure specifications provided by Purdue (< 200 psig). **Completed**

Green = completed. Brown = in progress.

4 – Progress and Accomplishments

Tasks 2.6, 2.7: Compositional and Physical Analysis

Task	Description	Status / Technical Accomplishments
2.6	Compositional analysis	**Milestone 2.6 (Initial results completed Aug 31, 2019; 18 mon from start); Compositional analysis continues through July 1, 2021:** • Ash content different between sheared (9.2%) and pelleted (15.6%) materials • Ash differences likely due to screening of fines
2.7	Physical analysis	**Milestone 2.7 (Aug 31, 2019; 18 mon from start) Physical Analysis continue through July 1 ,2021:** Sampling and sub-sampling protocols: • Size, shape, and density of sheared and pelleted materials complete • Pellet breakage model parameters measured • Completed tests for 3 out of 6 modified Drucker Prager Cap parameters at 3 different moisture contents

Green = completed; Brown = in progress

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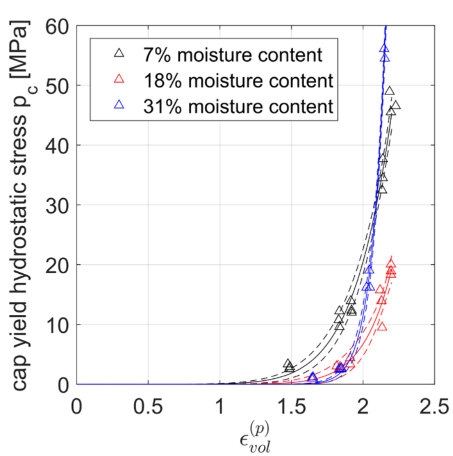
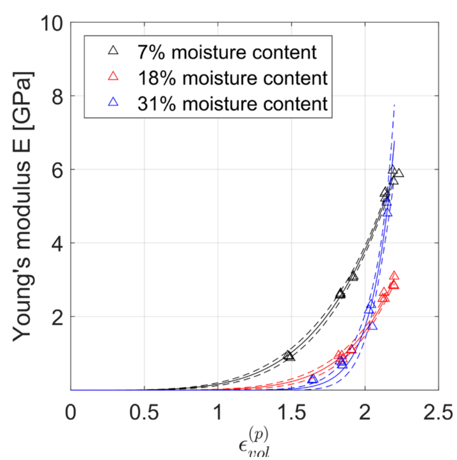
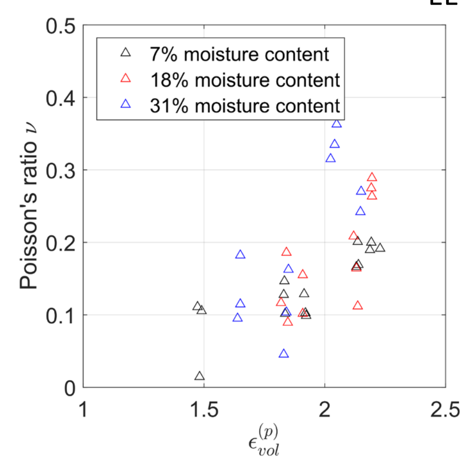


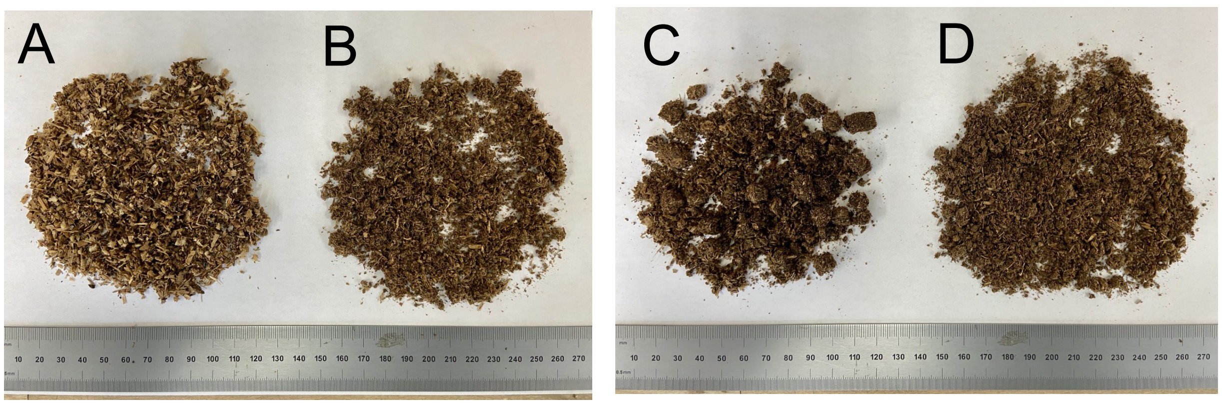




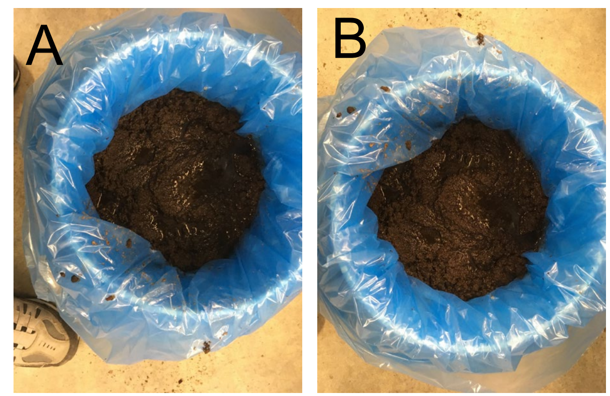
4 – Progress and Accomplishments

Tasks 3.1, 3.2: Batch process Development, Liquefaction

Task	Description	Status / Technical Accomplishments
3.2	Prep liquefied corn stover	**Milestone 3.1 (May 31, 2019; 25 mon from start); Development continues through Q3, 2021:** Preparation of intermediate liquefied corn stover at INL PDU *using aggregate corn stover material formed by feeding rotary sheared corn stover through the plug screw feeder.*
3.2	Prep liquefied corn stover	**Milestone 3.2 (18 and 21 mon from start): Development continues through Q3, 2021:** Preparation of intermediate liquefied corn stover at INL PDU *using aggregate corn stover material formed by feeding pelleted corn stover through the plug screw feeder.*



A) Loose, rotary sheared corn stover; B) Aggregate corn stover material prepared by feeding rotary sheared corn stover through the plug screw feeder; C) Loose corn stover pellets; D) Aggregate corn stover material prepared by feeding pellets through the plug screw feeder.



Intermediate liquified corn stover produced in the INL PDU from aggregates from A) rotary sheared material and B) pelleted material. Both prepared at 150ºC for 30 min, 40 mM maleic acid, 300 g/L solid.

4 – Progress and Accomplishments

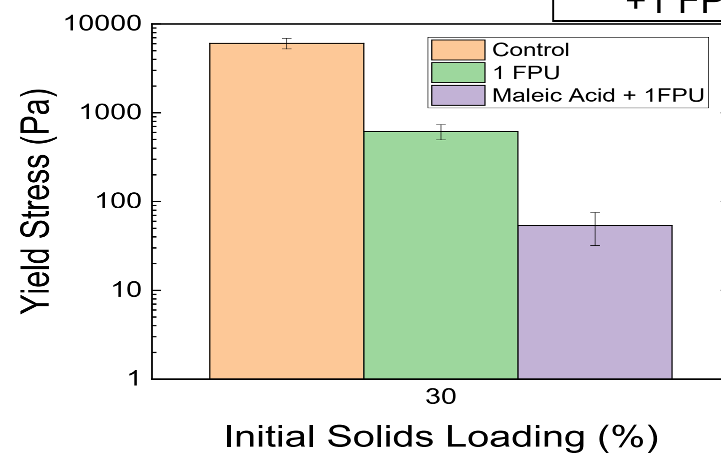
Tasks 3.1, 3.2 Batch process Development, Liquefaction

Task	Description	Status / Technical Accomplishments
3.1	Batch process development experiments New Since BP 1 Review	**Milestone 3.1 (May 31, 2019; 15 mon from start):** Batch process development experiments continue through Q3, 2021 • Rotary sheared stover laboratory-scale maleic acid liquefaction at Purdue • Rotary sheared stover laboratory-scale enzymatic liquefaction at Purdue • Pelleted stover laboratory-scale maleic acid liquefaction at Purdue • Pelleted stover laboratory-scale enzymatic liquefaction at Purdue • Pelleted stover lab-scale combined maleic acid/enzyme liquefaction @PU
3.2	Prep liquefied corn stover New Since BP 1	**Milestone 3.2 (July 31, 2019; 18 and 21 mon from start):** Preparation of intermediate maleic acid liquefied corn stover at INL PDU using pelleted corn stover continue through Q3, 2021

Corn stover Pellets needed for high % wgt / vol slurries

% Solids (w/v)	30	30	25 → 30
Celluclast 1 FPU/g solids 2.2 mg protein/g solids	No	Yes	Yes (Second)
40 mM Maleic Acid	No	No	Yes (First)
Time (Hours)	6	6	0.5 → 6
Temperature (°C)	50	50	150 → 50
Scale (mL)	300	600	30 → 600

Control | 1 FPU | Maleic Acid +1 FPU



4 – Progress and Accomplishments

Tasks 3.3, 3.4: Verification; Preparation of liquefied stover at INL

Task	Description	Status / Technical Accomplishments
3.3	Verification of modeling Results	**Milestone 3.3 (Sept 30, 2021; 24 months from start):** Batch process development experiments • Rotary sheared stover laboratory-scale maleic acid liquefaction at INL • Rotary sheared stover laboratory-scale enzymatic liquefaction at Purdue (subject to change order: focus on pellets) • Pelleted stover laboratory-scale maleic acid liquefaction at INL • Pelleted stover laboratory-scale enzymatic liquefaction at Purdue
3.4	Prep liquefied corn stover New Since BP 1 Review	Milestone 3.2 (after July 31, 2019; 18 and 21 mon from start): Preparation of intermediate liquefied corn stover at INL PDU Completed

Green = completed. Brown = in progress.

4 – Progress and Accomplishments

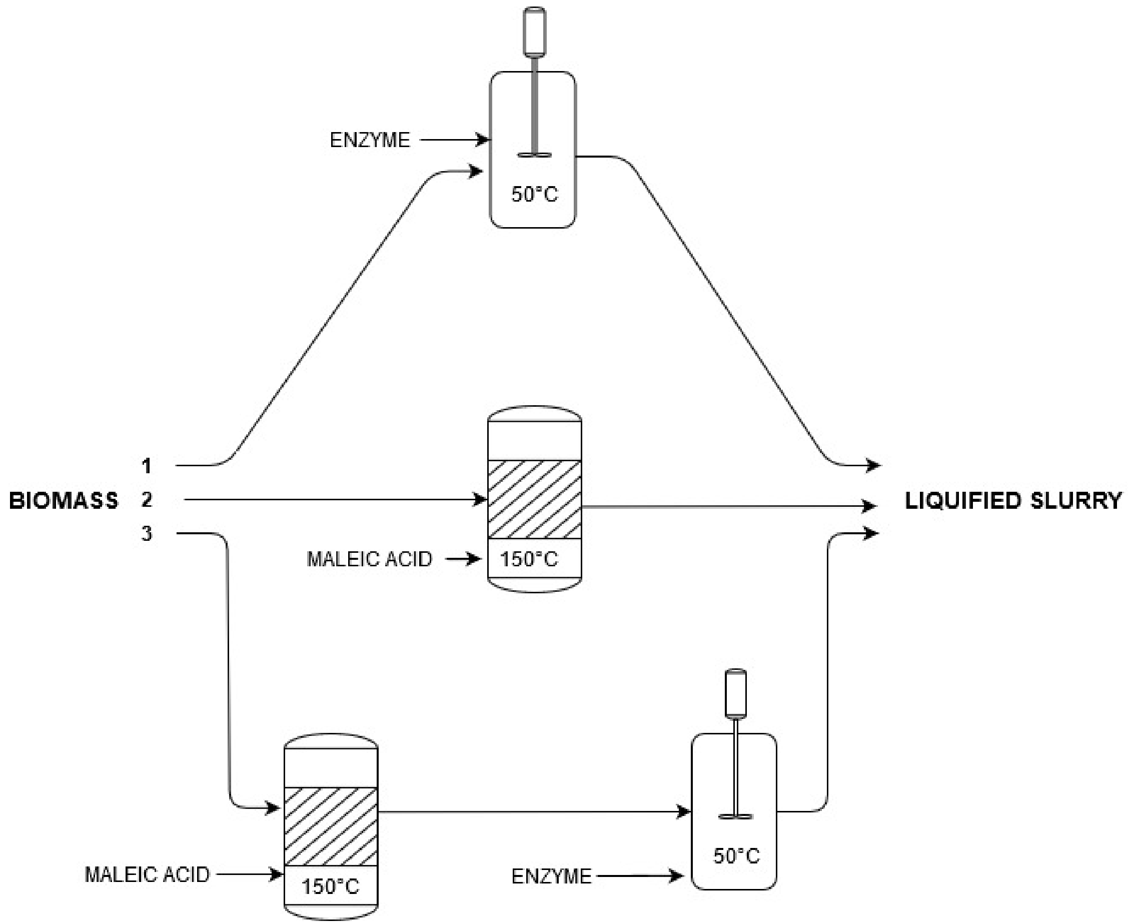
Tasks 4.1, 4.2: Verification; Preparation of liquefied stover at INL

Task	Description	Status / Technical Accomplishments
4.1	Preliminary Technical and economic assessment	**Milestone 4.1 (Oct 31, 2020; March 31, 2021 24 and 30 months from start):** Rotary sheared stover laboratory-scale maleic acid liquefaction at INL • Develop initial flowsheets based on modeling and verification results • Obtain data and information from different tasks to enable mass and energy balances to be calculated • Compare to industrial data (AdvanceBio)
4.2	Final Technical and economic assessment	Milestone 4.2 (June 30, 2021 30 months from start): Complete TEA, LCA for battery limits that define the preprocessing step investigated by this project, Limit analysis to this first steps that precedes pretreatment and subsequent biorefinery steps

Green = completed. Brown = in progress.

4 – Progress and Accomplishments

Tasks 4.1, 4.2: Verification; Preparation of liquefied stover at INL

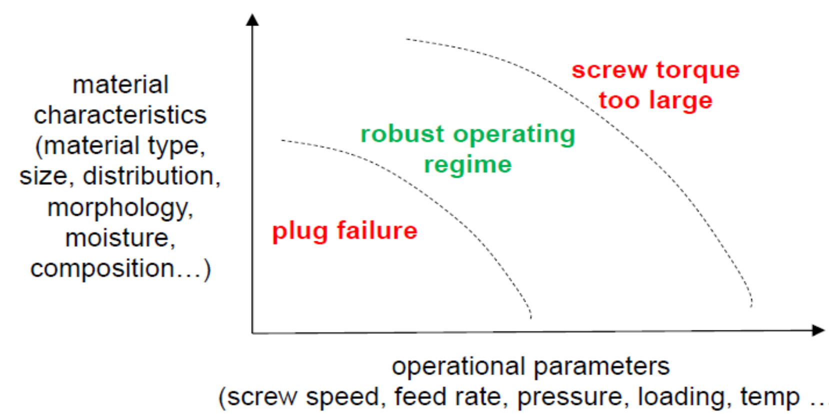


5 – Future Work

Task	Description	Next Steps
1.2	FEM modeling	• Parametric studies with the FEM model will be performed to identify operational regimes of compression feed screw and study sensitivity to mDPC parameters • Analytical models will be used to predict torque and plug density
1.3	CFD modeling	• Set up CFD model of reactor system • Identify rheological model for material behavior
2.1	Corn stover procurement and supply	• Continue to store corn stover for project duration. Supply formatted/preprocessed corn stover to Purdue on request as resources/testing requires.

5 – Future Work

Task	Description	Next Steps
2.6	Compositional analysis	• Complete the compositional analyses of the Forest Concepts and INL processed materials (beyond ash) to understand inherent variation of process inputs
2.7	Physical analysis	• Conduct initial characterization of rheological properties of corn stover slurries as a function of solids loading and liquefaction. • Work with Forest Concepts/Penn State team to obtain DEM calibration and FEM DPC measurements • Measure material-wall friction angle
3.1	Batch process development experiments	• Perform laboratory scale enzymatic and maleic acid liquefaction of pelleted corn stover at bench scale.
3.3	Verification of modeling results	• Production of maleic acid liquified material from pelleted corn stover in reactor pressurized specifications provided by Purdue (< 200 psig) at a 1 ton (dry weight) per day scale.
4.1	TEA and LCA models	• Carry out TEA around flowsheet for feed / compression section. Inputs and operational envelope based on DEM, FEM and CFD models • Carry out LCA based on TEA



Summary

Overview: Addresses major impediment to reliable biorefinery operation, moving solids from one unit operation the next.

Approach: Develop fundamental mathematical models, verified in INL pilot facility, that predict transport of corn stover particles and slurries at high solids loadings between biorefinery unit operations

Technical Accomplishments. FEM simulations were optimized, and partial calibration of model was done for different moisture contents. Did preliminary work on a concise semi-analytical model. Concept of liquefaction demonstrated for enzyme and maleic acid (enzyme biomemetics). Verification runs in process. 30 % w / vol achieved.

Relevance: Usable, scientifically-based computational tools for process analysis that simplify process design, enhance operational reliability, and reduce capital and operating expenses. Supports BETO's mission and MYPP.

Future Work: Perform FEM parametric studies, construct operational regime maps and build a semi-analytical model; and identify rheological behavior of corn stover slurries at loading at up to 300 g/L. Laboratory measurements to be validated against mathematical models and INL pilot tests.

Calibrate models against measured physical parameters for pelleted and particulate corn stover feedstocks; parametric simulations; Validate measured properties for corn stover against mathematical models.

Additional background materials:

- Quad chart
- High level Gantt chart
- Risk Mitigation
- Publications

Quad Chart Overview: EE 0008256

Timeline

- Project start date: - March 1, 2018
- Project end date – Sep 30, 2021

	FY20 Costed	Total Award
DOE Funding	(10/01/2019 – 9/30/2020) *$356,355*	$1,190,000
Project Cost Share	$333,210	$519,822

Project Partners* Led by Purdue Uni.

- Partner 1: INL
- Partner 2: ANL
- Partner 3: AdvanceBio
- Partner 4: Forest Concept

*Only fill out if applicable.

Project Goal

(1) Develop strong and innovative computational models that rigorously represent flow performance of biomass materials; (2) Verify models in cooperation with the Idaho National Laboratory using INL pilot scale equipment; (3) Support technology development and engineering solutions that economically and sustainably overcome critical barriers associated with handling of solids in biorefinery production process.

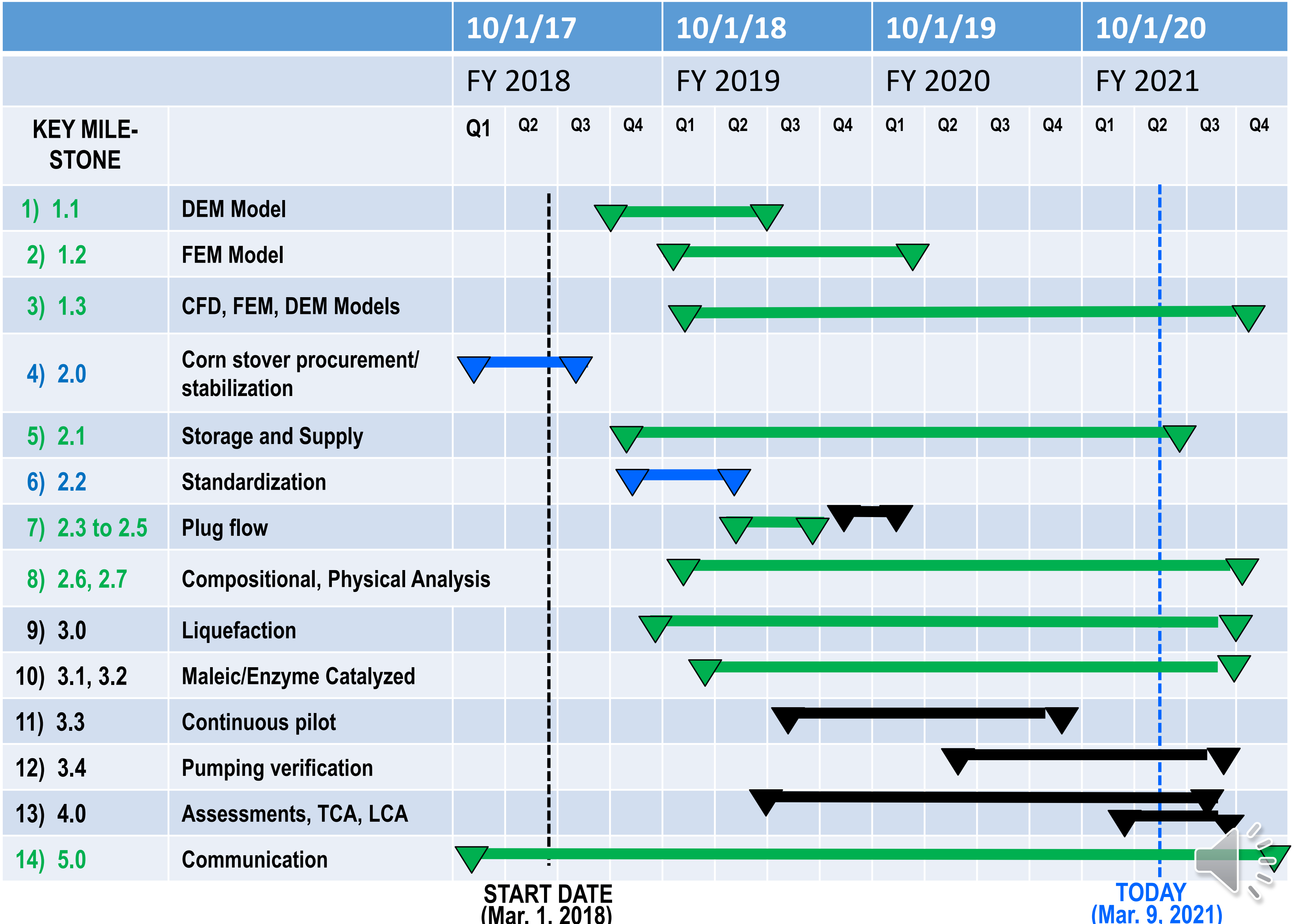
End of Project Milestone

Demonstration of effective models for accurately predicting/simulating flow of biomass solids, and specifying operational envelope for stable flow of biomass solids through a compression screw feeder, horizontal screw reactor, and slurry pump. The objective is to calculate and verify the model for a target concentration in the range of 150 to 300 g/L solids, between ca. 20 and 80% of maximum throughputs of the feeder or pump, a temperature of between 50 and 160°C, and solids particles consisting of either loose (ground corn stover, rotary sheared) or corn stover pellets (hammer milled and then pelleted) as defined in the proposal narrative.

Funding Mechanism

DOE-FOA-0001689
Advanced Development and Optimization

Milestones – Analytical Modeling EE0008256



Project Risks and Mitigation

Risks:

Models do not function (predict) as expected based on verification (experiments) that show models must be adjusted.

Mitigation:

Twice per month teleconferences with project partners

Executive team call

Once per 2-month call with program manager and project monitor

Purdue research meeting every 4^{th} Tuesday

Purpose is to chart technical progress, discuss options / midcourse corrections

Stakeholder conference planning (virtual meeting) March / April 2021

Publications, Patents, Presentations, Awards, and Commercialization

Publications / Presentations:

- Almeida R.M.R.G., Pimentel W.R.O., Santos-Rocha M.S.R., Buffo M.M., Farinas C.S., Ximenes E.A., Ladisch M.R. Protective effects of non-catalytic proteins on endoglucanase activity at air and lignin interfaces. *Biotechnology Progress* (2021e3134. doi: 10.1002/btpr.3134. Online ahead of print.
- Ximenes E., Farinas C., Baldino A., Ladisch M. Moving from residual lignocellulosic biomass into high-value products: outcomes from a long-term international cooperation. *Biofuels, Bioproducts & Biorefining* (Early access, DEC 2020).
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