DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Analytical Modeling of Biomass Transport and Feeding Systems

EE0008256

WBS 3.5.3.4

March 7, 2019

Technology Session Area Review

Advanced Development and Optimization

Michael Ladisch, Carl Wassgren, Nathan Mosier, David Thompson, Pankaj Sharma, Jim Dooley, Dale Monceaux, Pahola Thathiana Benavides Gallego, Marcial Gonzalez, Tyler Westover, Eduardo Ximenes, Kingsly Ambrose, Klein Ileleji, John Aston, Abigail Engelberth

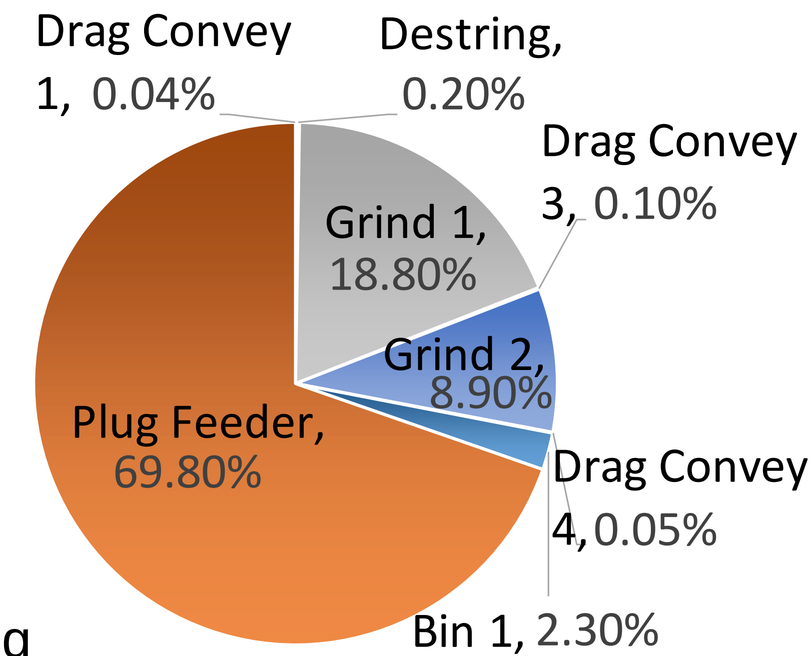
Collaborators: INL, ANL, Forest Concepts, AdvanceBio, Penn State

Goal Statement

Analytical modeling that rigorously represents flow performance of biomass materials at high solids loading, based on fundamental mathematical models:

Predict flowrates as a function of torque for particulate and pelleted forms of corn-stover for a tubular pretreatment reactor (CPS), and

Application of models to calculate operation envelopes.



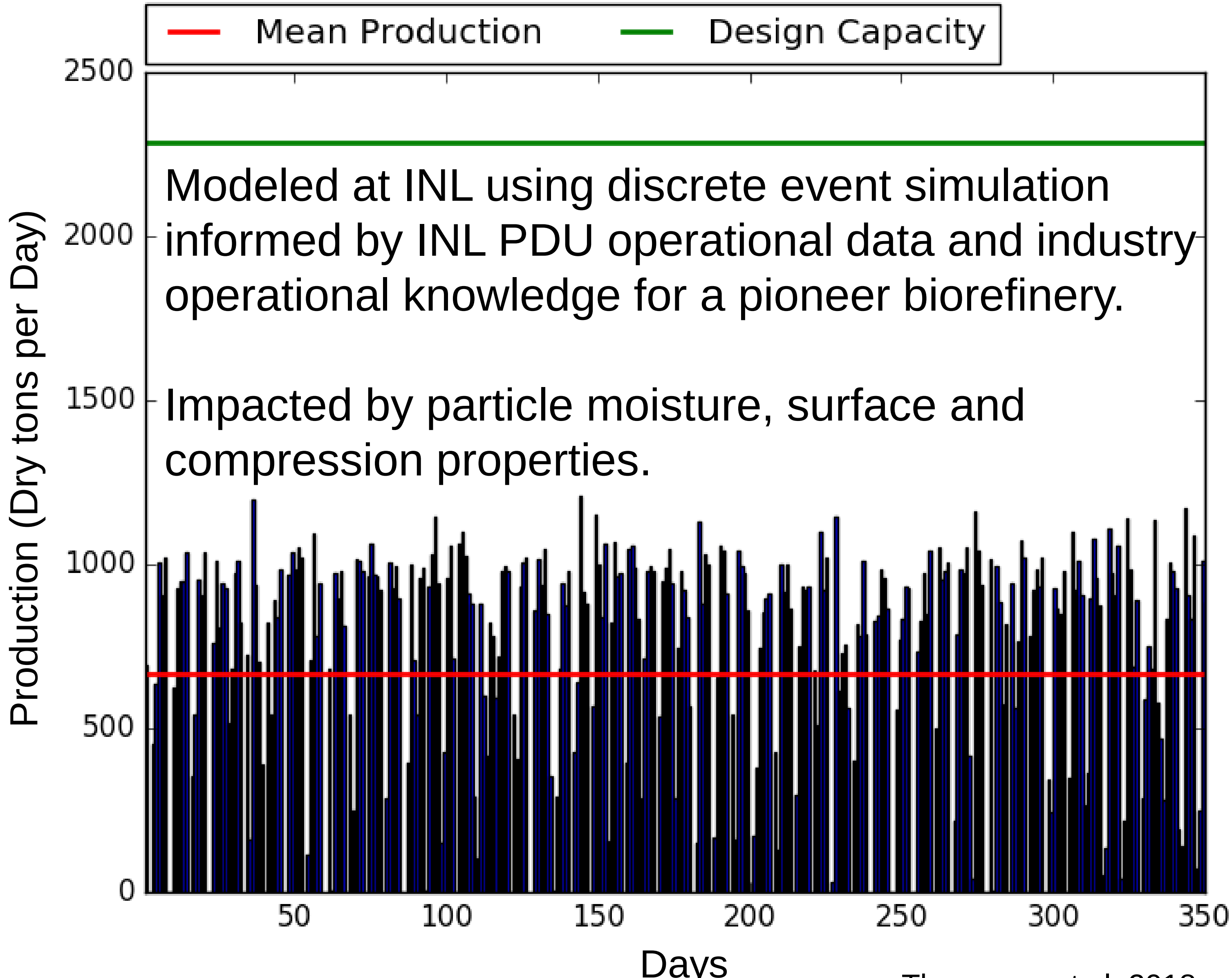
Relevance and Tangible Products for US:

Predictive models that define conditions for robust operation and minimize downtime in biorefineries due to plugging by pumping and mixing of biomass.

Usable, scientifically-based computational tools for process analysis to simplify process design.

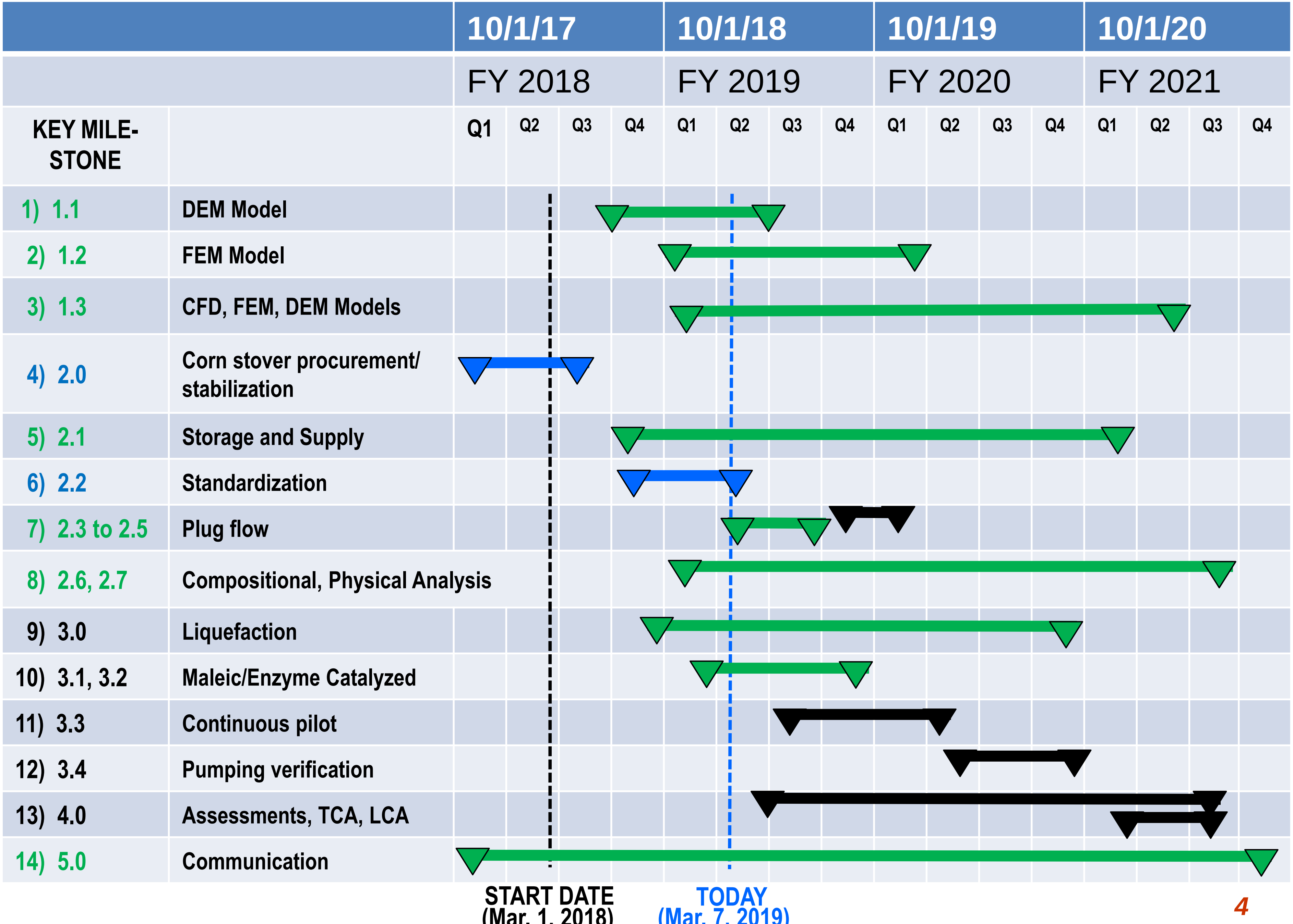
Enhance operational reliability, and reduce capital and operating expenses.

Technical Challenge: Economic Impact



Thompson et al. 2018

Key Milestones – Analytical Modeling EE0008256



Purdue Project Budget Table by Budget Period and Task

	Original Project Cost (Estimated)			DOE Project Spend and Balance		Final Project Costs
Budget Periods	**DOE Funding**	**Project Team Cost Shared Funding**	**Contin gency.**	**DOE Spending to Date**	**DOE Remaining Balance**	**Funding needed to complete project**
BP 1 Mar. 1, 18 to Feb. 28, 19			N/A			
Task 1 Modeling	148,685	43,069		20,590	128,095	0
Task 2 Characterization	238,915	69,206		293,373	(109,812)	0
Task 3 Verification	37,130	10,755		20,053	17,077	0
Task 4 Assessment	24,215	7,014		1,000	24,215	0
Task 5 Communications	53,884	15,608		17,198	19,853	0
BP 2 Mar. 1, 19 to Feb. 28, 20			N/A			
Task 1	125,792	3,6438		0	125,792	0
Task 2	186,116	5,3912		0	186,116	0
Task 3	180,407	52,258		0	180,407	0
Task 4	78,961	22,873		0	78,961	0
Task 5	66,809	19,352		0	66,809	0
BP 3 Mar. 1, 20 to Feb. 28, 21			N/A			
Task 1	178,612	51,738		0	178,612	0
Task 2	126,781	36,724		0	126,781	0
Task 3	183,795	53,240		0	183,795	0
Task 4	106,214	30,767		0	106,214	0
Task 5	63,684	18,447		0	63,684	0
Total	1,800,000	521,403		352,214	1,447,786	0

Quad Chart Overview: EE 0008256

Timeline

Project start date: Mar 1, 2018
Original end date: Feb 28, 2021
Revised end date: Sept 30, 2021
since funds obligated Mar 1, 2018
Status: 19% complete (Q2 FY 19)

Barriers Addressed

FSL-PM7 MYPP. *Terrestrial Feedstocks*
Validate cellul. feedstock supply (2021)

Ft-H Barrier. *Terrestrial Feedstocks.*
Biomass handling / transport

FT-G Barrier. *Terrestrial Feedstock*
Biomass physical size alteration.

FT-J Barrier. Operational reliability.

Budget

	Total Costs Pre FY 17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
Purdue Expenditure (DOE Funded)	0	0	184,472	1,005,528
Purdue (Cost-share)	0	0	4,313	462,375
Forest Concepts (Cost Share)	0	0	27,229	2,486
AdvBio (Cost-Share)	0	0	8,600	16,400
INL	0	0	119,561	430,439
Argonne	0	0	1,000	59,000

Partners

National Laboratories (% of DOE funds)

Idaho National Laboratory (INL) 30.6
Argonne National Lab (ANL) 3.3

Other interactions / Collaborations
Forest Concepts LLC 5.0

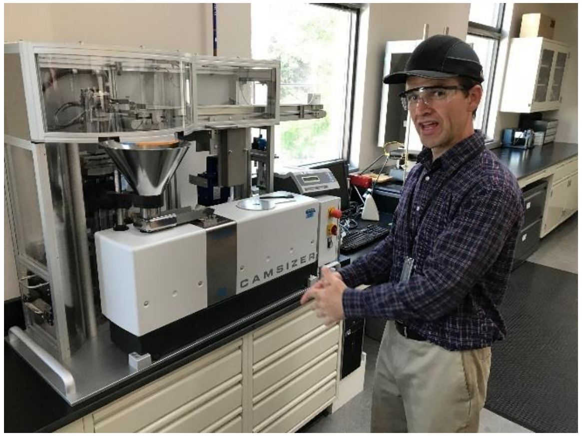
AdvanceBio - Engineering
Penn State – compaction analysis / research discussions
DOE program managers

1 - Project Overview

Analytical Modeling of Biomass Transport and Feeding Systems
(EE 008256)

Project goals are:

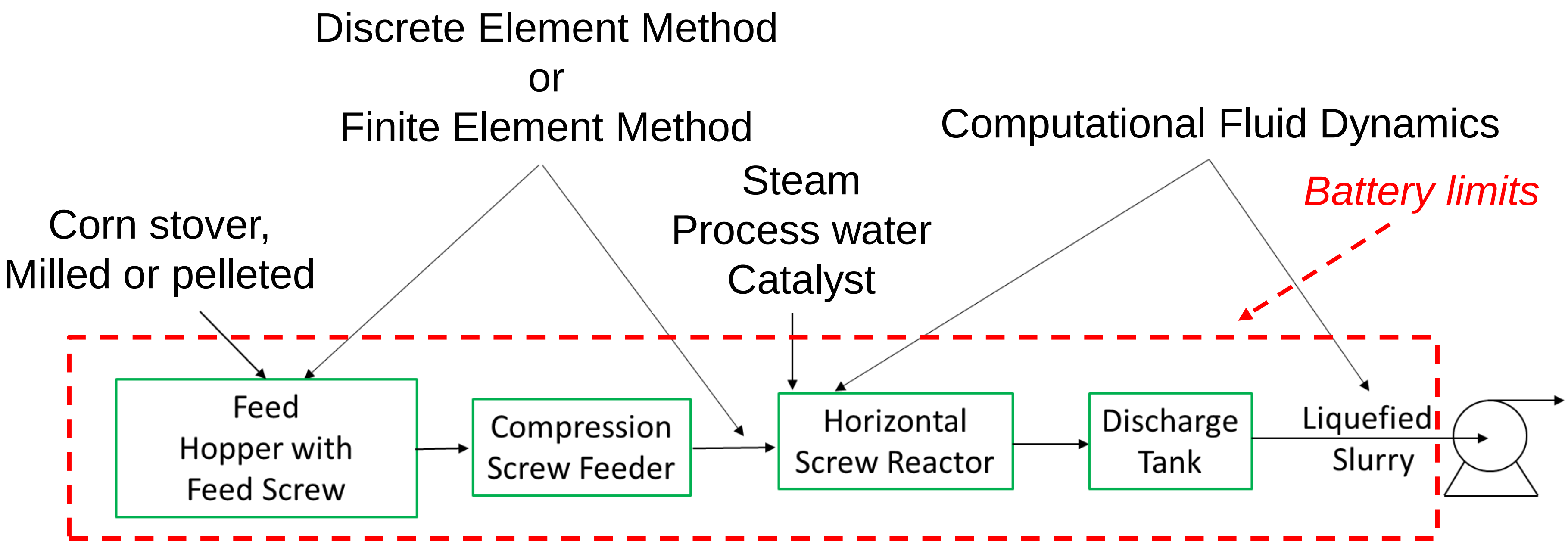
- Develop strong and innovative computational models that rigorously represent flow performance of biomass materials.
- Verify models in cooperation with the Idaho National Laboratory using INL pilot scale equipment.
- Support technology development and engineering solutions that economically and sustainably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

2 – Approach (Technical)

- 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

Process Operations Block Diagram



Feedstock, material and energy input

GHG emissions
FFC consumption
Water consumption

2 – Approach (Management)

Michael Ladisch
Project Director

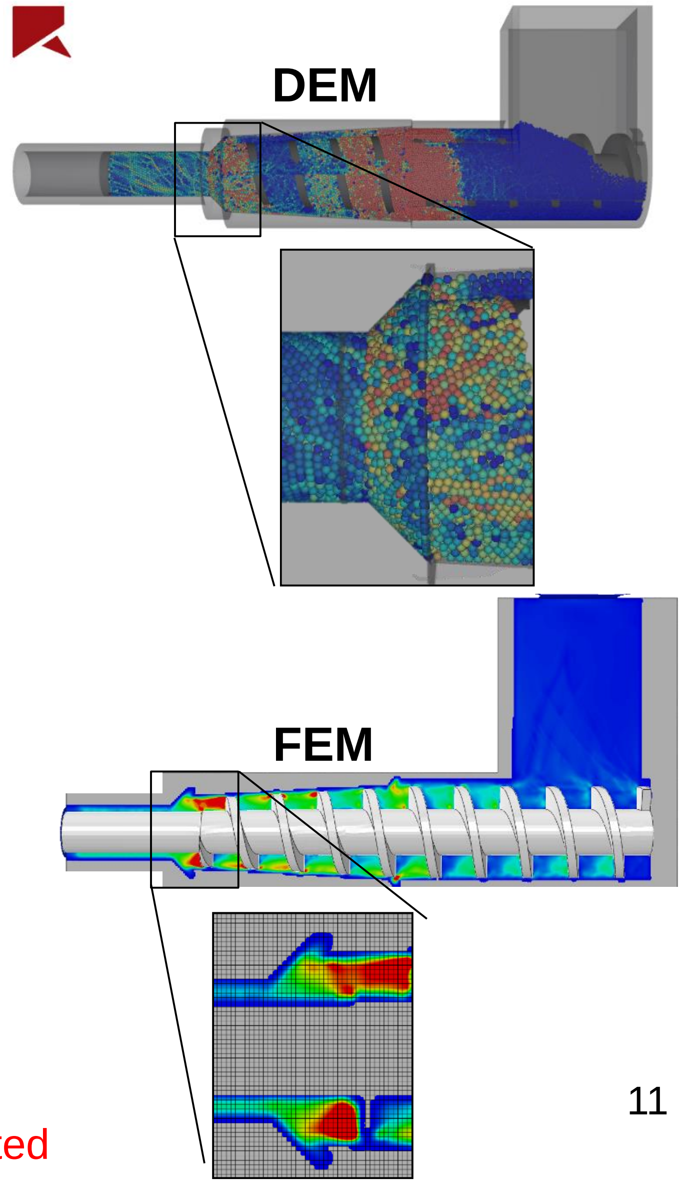
Carl Wassgren,
David Thompson, Nathan Mosier
Pankaj Sharma
Project Co-Directors

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

3 – Technical Accomplishments/ Progress/Results

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	• Compression screw model setup complete • Measurement methods setup complete • Constitutive models incorporated **Go/No-Go Decision Pt 2 (anticipated April 1, 2019, 13 months from start):** FEM software operational, demonstrated preliminary model with ground corn stover feeding (in progress)
1.3 CFD modeling	**Milestone 1.1.3 (Feb 1, 2019, 11 months from start; not completed)** : CFD modeling software installed and modeling initiated

Green = completed; Brown = in progress; Red = not completed



3 – Technical Accomplishments/ Progress/Results (cont.)

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; not completed) ; 6, 18, 30 months from project start):** Standardization completed at INL; corn stover feed plug delivered to Purdue for analysis.

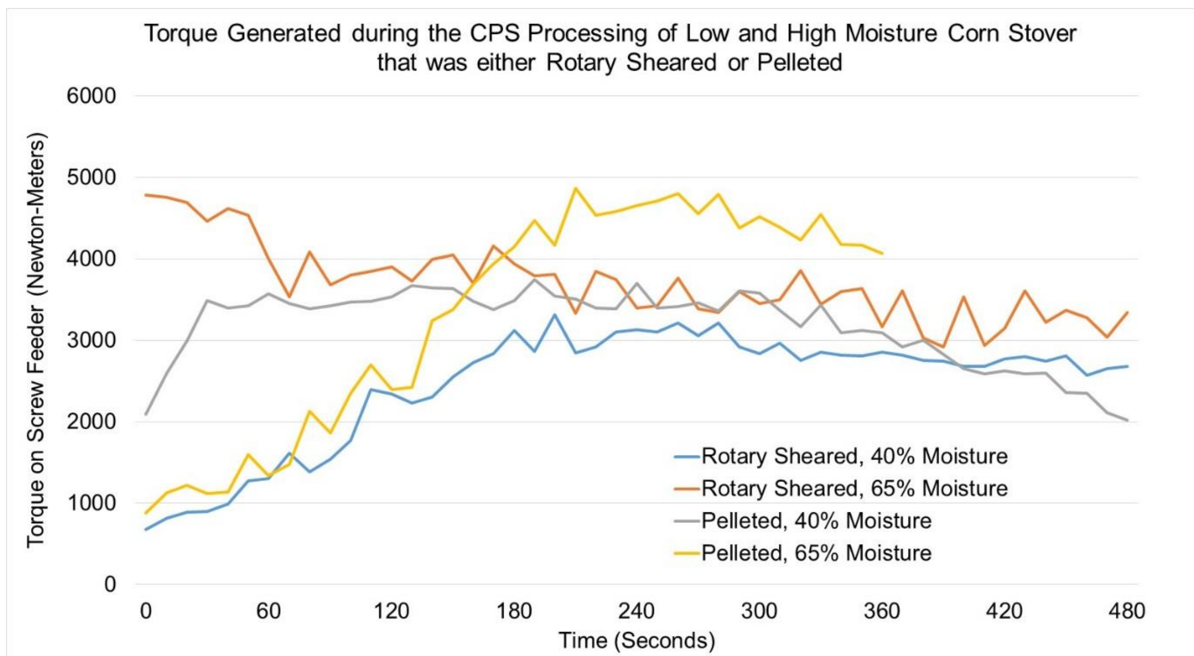



Green = completed. Brown = in progress. Red = not completed.

3 – Technical Accomplishments/ Progress/Results (cont.)

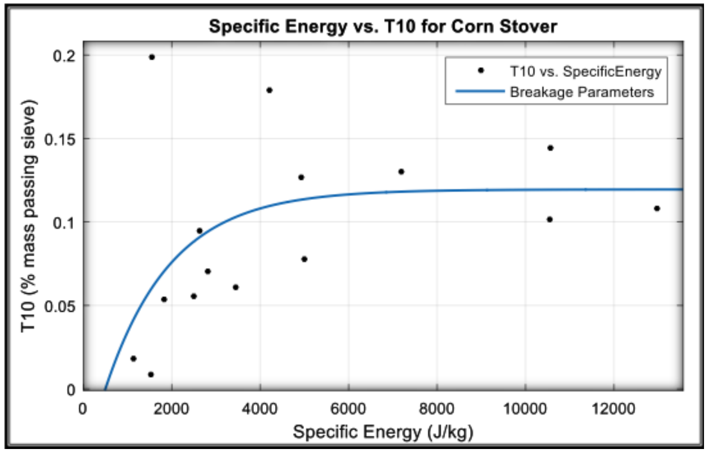
Task	Description	Status / Technical Accomplishments
2.3	Plug flow testing	**Milestone 2.3.1 (Dec 1, 2018; 9 months from project start):** Formation of plug with rotary sheared stover **Milestone 2.3.2 (Dec 1, 2018; 9 months from project start):** Formation of plug with pellets Materials at 40% and 65% moisture content
2.4	Verification of plug integrity in pressurized reactor	**Milestone 3.2 (after July 31, 2019; 6, 18 and 21 mon from start)** with rotary sheared and pelleted corn stover **Milestone 2.4.2:** with pelleted stover

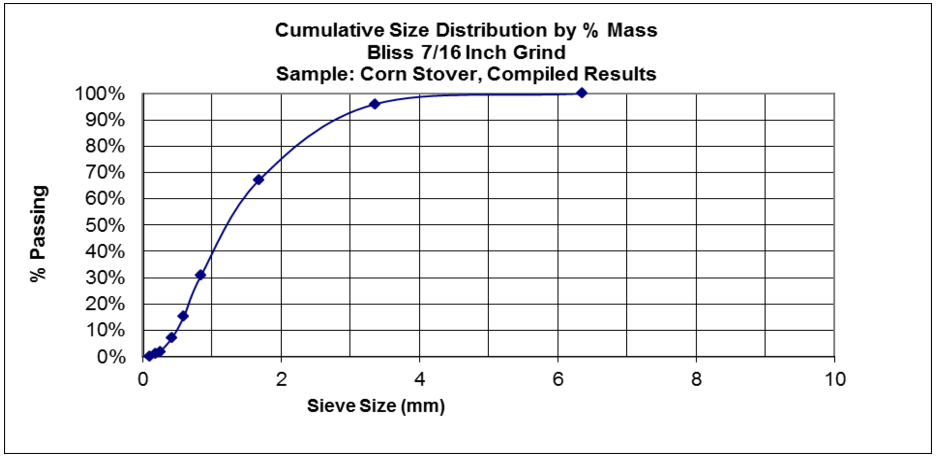
Green = completed
Brown = in progress
Red = not completed



3 – Technical Accomplishments/ Progress/Results (cont.)

Task	Description	Status / Technical Accomplishments
2.6	Compositional analysis	**Milestone 2.6 (Aug 31, 2019; 18 mon from start):** Compositional analysis • 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 analyses • Sampling and sub-sampling protocol established • Size, shape, and density of sheared and pelleted materials complete • Pellet breakage model parameters measured • Partnering with Forest Concepts/Penn State team to obtain sheared stover Drucker Prager Cap parameters obtained from a cubical triaxial tester

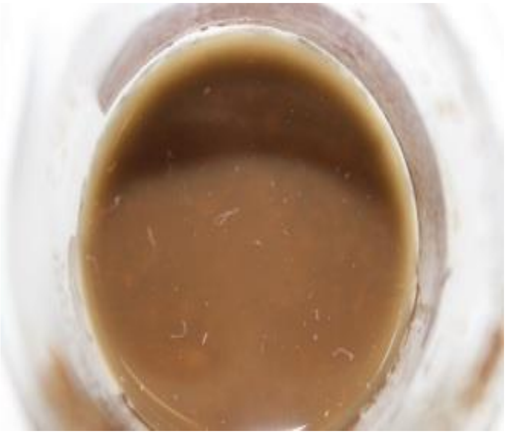




Brown = in progress

3 – Technical Accomplishments/ Progress/Results (cont.)

Task	Description	Status / Technical Accomplishments
3.1	Batch process development experiments	**Milestone 3.1 (May 31, 2019; 15 mon from start)**: Batch process development experiments • 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
3.2	Prep liquefied corn stover	**Milestone 3.2 (after July 31, 2019; 18 and 21 mon from start)**: Preparation of intermediate liquefied corn stover at INL PDU



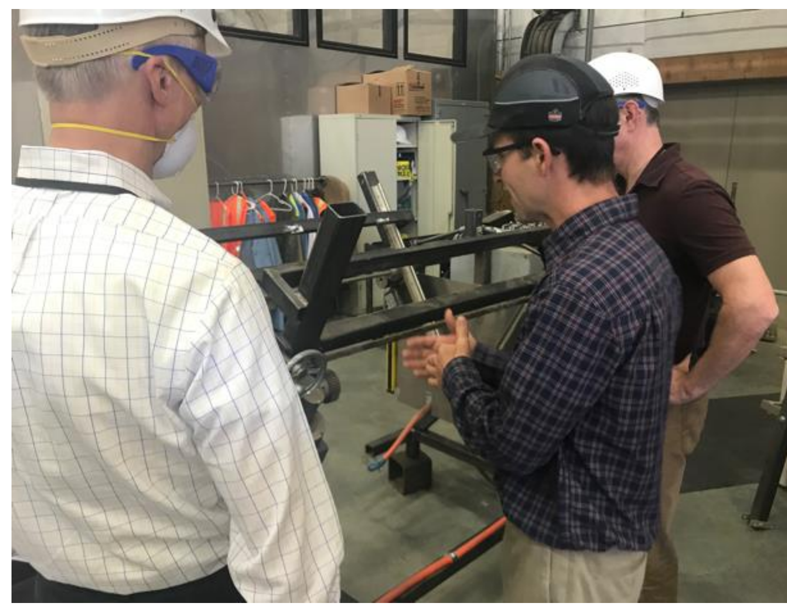
Enzyme liquefied (300 g stover / L, 10 h, 50°C)

150 g stover /L, 30 min,150°C
13 mM Maleic acid

Green = completed. Red = not completed.

3 – Technical Accomplishments/ Progress/Results (cont.)

Task	Description	Status / Technical Accomplishments
5	Communications	**Milestone 5.1 (submitted Oct 31, 2018):** 1st Quarterly Review Report **Milestone 5.2 (Submitted Jan 30, 2019):** 2nd Quarterly Review Report • Twice per month teleconferences with project partners • Purdue content sharing site operating (PURR) • Once per month call with program manager and project monitor



Relevance

Directly supports BETO’s mission

IBR development and operation that accounts for complexity and variability of lignocellulosic biomass, inconsistent feeding and handling, equipment design, and flawed integration. Achieve cost effective operation with > 90% on-stream reliability. Fundamental R&D that identifies key feedstock quality and operational factors affecting operational reliability and addresses process or operational strategies that mitigate remaining factors.

Addresses BETO’s MYPP goal

“to develop and validate feedstock supply to support a biorefining industry,” … and addresses the barrier of *“providing computational tools that inform designs and conditions for grinding, sizing, and moving cellulosic biomass materials so that they are transported from one unit operation to another without plugging, leading to reliable plant operation.”*

Addresses Barriers

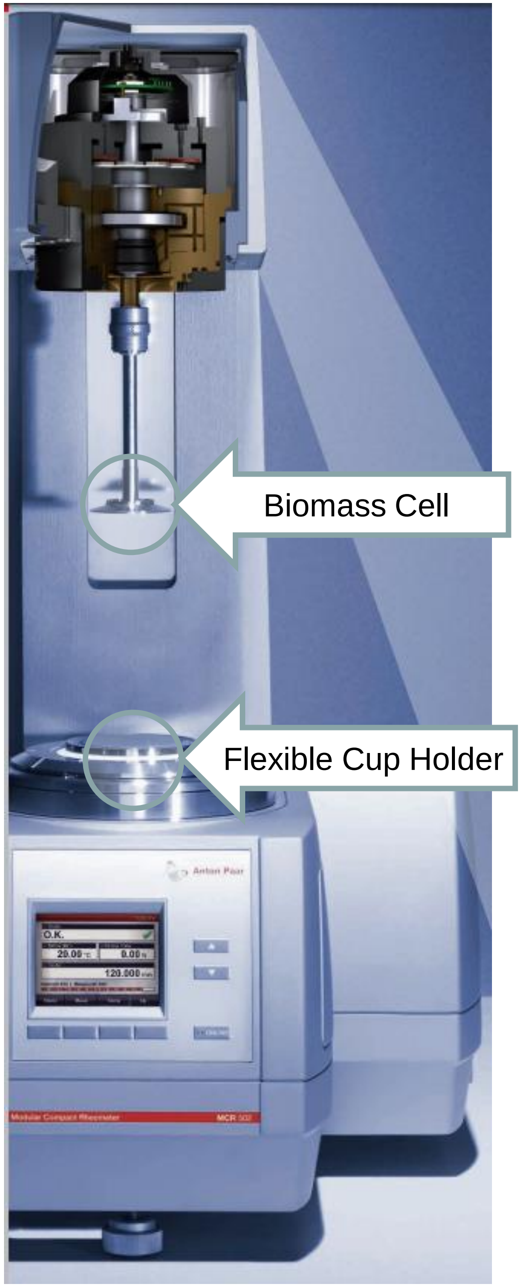
FSL-PM7 MYP.
Terrestrial Feedstocks
Validate cellulose feedstock supply (by 2021)

Ft-H Barrier.
Terrestrial Feedstocks.
Biomass handling / transport

FT-G Barrier.
Terrestrial Feedstock
Biomass physical size alteration.

FT-J Barrier.
Operational reliability.
Account for complexity of lignocellulosic biomass.
Cost effective operation.
> 90% on-stream reliability.

5 – Future Work – Computational Fluid Dynamics Modeling



Biomass Cell
- Allows for continuous sample mixing to avoid sedimentation

Flexible Cup Holder
- Analyze variation in flow with sample cell dimensions

Rotational Rheometry (Erk and Szeto, Purdue MSE)

- Rheometry measurements on wet biomass slurries will be used to verify/validate the predictions from modeling efforts.
- End goal is to determine characteristics of biomass and/or processing parameters that result in a pumpable slurry.

<u>Key Rheometry Measurements</u>

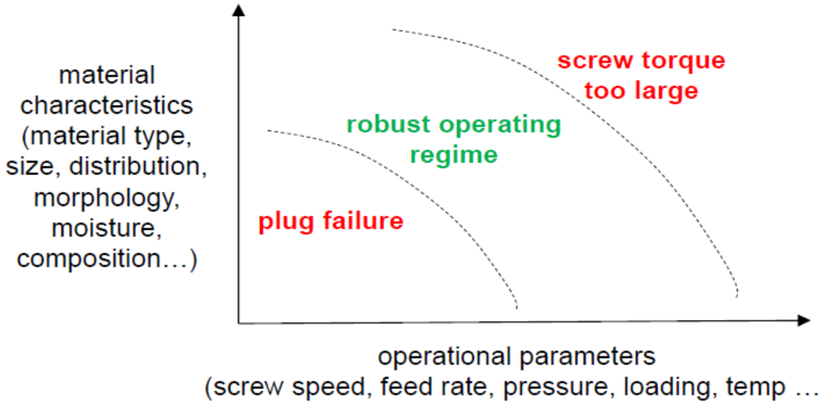
- **Viscosity**– fluid property of resistance to flow
- **Flow Curve** – identify non-Newtonian behavior with changes in shear rate
- **Yield Stress** – reveal minimum pump power requirements to induce flow
- **Thixotropy** – detect changes in flow behavior over time

5 – Future Work

Task	Description	Next Steps
1.1	DEM modeling	• Calibrate DEM material and interaction properties against Cubical Triaxial Tester (CTT) experimental data and wall shear tests • Perform parametric simulations to measure mass flow rate, screw torque, and stresses as a function of screw speed and variations in material properties • Go-No Go Decision (April 1, 2019; 13 months from project start): Comparison of DEM model predictions against experimental screw torque measurements
1.2	FEM modeling	• Include material hardening behavior into DPC constitutive model • Obtain DPC properties from CTT experimental data • Perform parametric simulations to measure mass flow rate, screw torque, and stresses as a function of screw speed and variations in material properties
1.3	CFD modeling	• Set up CFD model of reactor system • identify rheological model for material behavior
2.3	Plug flow testing	• Validate/adjust CPS operating/feedstock parameters developed under ambient conditions to successfully process rotary sheared and pelleted corn stover in a pressurized system. • Collect inlet/outlet to support the project's analyses and modeling tasks. • Key milestones: Q2, FY19: Verification of Plug Integrity in Pressurized Reactor Determine the suitability of plugs formed in the CPS under pressurized reactor conditions Assign an approximate "pressure rating Q3, FY19: Production of Plug Material in Pressurized Reactor Produce formed plugs and provide them to Purdue

5 – Future Work (cont.)

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.
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. Initial computations using DEM and FEM models completed. Concept of liquefaction demonstrated.

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: Calibrate models against measured physical parameters for pelleted and particulate corn stover feedstocks; perform parametric simulations; and identify rheological behavior of corn stover slurries at loading of 150 to 250 g/L. Laboratory measurements to be validated against mathematical models and INL pilot tests.

Additional Slides

Responses to Previous Reviewers' Comments

No prior reviews carried out for this project.

Consequently, no response is offered

Publications, Patents, Presentations, Awards, and Commercialization

Publications / Presentations:

dos Santos, A-C., E. Ximenes, Y. Kim, and M. R. Ladisch, "Lignin-Enzyme Interactions in the Hydrolysis of Lignocellulosic Biomass," Trends in Biotechnology (published on-line, Dec. 2018; doi.org/10.1016/tibtech.2018.10.010).

Ladisch, M., "Biorefining: Engineering, Science, and Economics," Academia Nacional Ingenieria, Uruguay 2018 CAETS, Montevideo, Uruguay (September 12, 2018).

Patents awarded in 2016 – 2018
(not funded by EE 0008236, but provide background for this project):

Stater, B., B. Spindler, C. Wyman, N. Mosier, M. Ladisch, "Process for Preparing Enriched Glucan Biomass Materials," Chinese Patent ZL201080046974.3 (December 7, 2016).

Publications and Patents (continued,

Patents awarded in 2016 – 2018 (continued)
(not funded by EE 0008236, but provide background for this project):

Ladisch, M. R., B. Stater, B. Spindler, “Locally-Regulated Pressurized Pretreatment of Lignocellulosic Biomass,” US Patent 9,777,341B2 (October 3, 2017).

Ladisch, M. R., E. Ximenes, T. R. Kreke, A. C. Badino, F. da Cunha, C. S. Farinas, “Liquefied Cellulosic Biomass for Enzyme Production,” US 10,072,253 B2 (September 11, 2018).

Ladisch, M. R. and Y. M. Kim, “Enzyme Catalyzed Disassembly of Corn Kernels,” US Patent 10,093,951 B2 (October 9, 2018).

Ladisch, M. R., B. Stater, B. Spindler, “Flow Process for Pretreatment of Lignocellulosic Biomass,” US Patent 10,125,454 B2 (November 13, 2018).

Ladisch, M. R., N. S. Mosier, Y. Kim, J. van Rooyen (Mascoma), “Liquefaction Biomass Processing with Heat Recovery,” US 10,144,785 B2 (December 4, 2018).

Describe the status of any technology transfer or commercialization efforts

Discussions underway or planned with several corn to ethanol biorefineries

Patent strategy is to develop a portfolio that will protect IP and thereby encourage commercialization of technology once research is complete

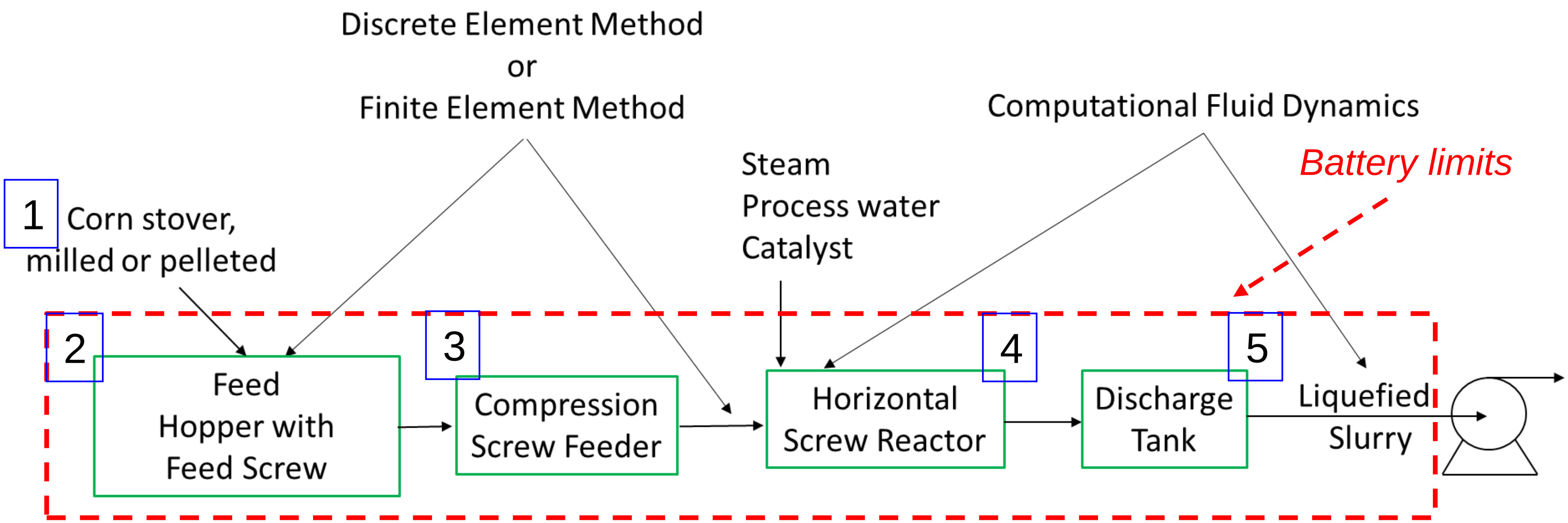
The major tool from this project is a mathematical model verified against existing system at INL – rather than construction of an actual system.

Units are already use in US and S. America at pilot scale (AdvanceBio that built these is a partner in this project).

Project Scope Change Table

Scope Changes	Date	Logic / Reasoning	Approval / Rejection Date
BP1			
No scope change	Dec 31, 2018	Not applicable – there is no change	Not Applicable
BP2 No scope Change	Jan 31, 2019	Not applicable - there is no change	Not Applicable

Process Operations Block Diagram



Process Risks: Risk Table

Risk ID		Risk Identified			Mitigation Strategy		
	Process Step	**Risk Described**	**Severity**	**Probability**	**Mitigation Response**	**Planned Action Date**	**Current Status**
Feed Preparation							
	1	Corn stover degrades	High	Low	Obtain new lot	None	Stover stabilized
Feed Hopper with Screw	2						
		Material does not convey	High	Low	use model to calculate screw rotation speed	None	Testing intiated
Compression feed screw	3						
		Compression screw jams	Low	High	Disassemble and clean; control CS particle size	Upon occurrence	Testing Initiated
Horizontal Screw Reactor	4						
		Screw reactor jams	Med	Low	Disassemble and clean; adjust % fill; speed, particle size	Upon occurrence	Testing will be initiated in FY19
Discharge Tank	5						
		Discharge Valves Plug	Med	Med	Disassemble and clear. Adjust discharge pressure actuators.	Q3 FY19	Not yet started

Process Risks: Risk Table

Risk ID		Risk Identified			Mitigation	Strategy	
	Process Step	Risk Described	Severity	Probability	Mitigation Response	Planned Action Date	Current Status
FEM	1	FEM model too time consuming	Med	High	Model simplifications	None	In-progress
	2	Material not properly calibrated	Med	Med	Partnership w/ Forest Concepts/Penn State	None	In-progress
	3	FEM model inaccurate	High	Med	Material property calibration; use of DEM	None	Not yet started
DEM	1	DEM model too time consuming	Med	High	Model simplifications	None	In-progress
	2	Material not properly calibrated	Med	Med	Partnership w/ Forest Concepts/Penn State	None	In-progress
	3	DEM model inaccurate	High	Med	Model calibration; use of FEM	None	Not yet started

Process Risks: Risk Table

Risk ID		Risk Identified			Mitigation Strategy		
	Process Step	Risk Described	Severity	Probability	Mitigation Response	Planned Action Date	Current Status
CFD	1	Rheological model inaccurate	High	Med	Test w/ various models	None	Not yet started
	2	CFD model too slow	Med	High	Model simplifications	None	Not yet started
	3	CFD model inaccurate	High	Med	Calibration of model parameters	None	Not yet started