DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Integrated Computational Tools to Optimize and De-Risk Feedstock Handling & High-Pressure Reactor Feeding Systems: Application to Red Rock Biofuels' Biorefinery (WBS 3.3.1.2)

Advanced Demonstration and Optimization: Analysis Modeling

7 March, 2019

Jonathan Stickel (presenter) and Peter Ciesielski

National Renewable Energy Laboratory

Goal Statement

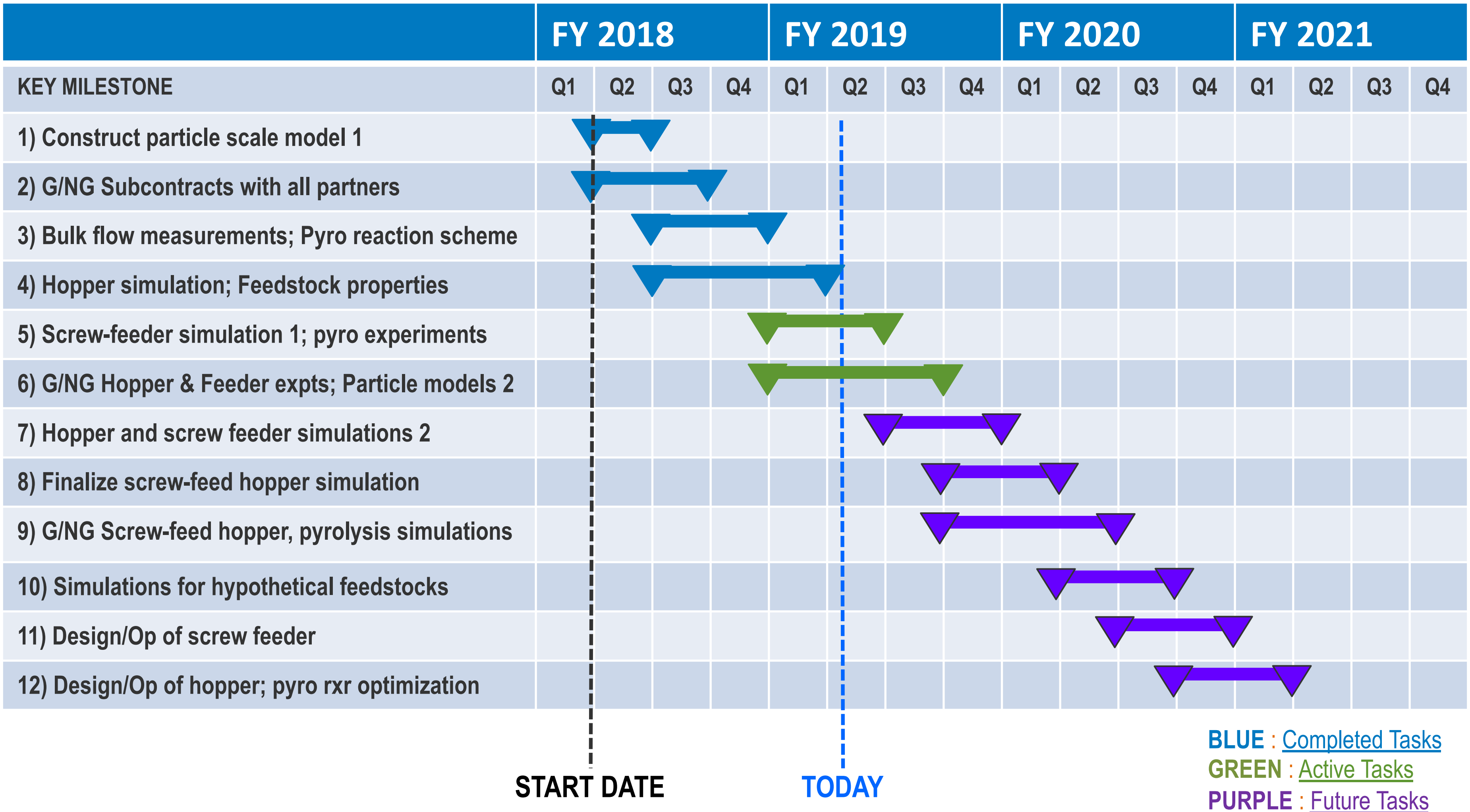
Goal: Develop robust physics-based models for the feed-handling unit operations at the front end of the Red Rock Biofuels' (RRB) gasification process and to experimentally validate these models at industry-relevant conditions.

Outcome: Optimized and reduced-risk deployment of an industrial biomass gasification process enabled by high-fidelity physics-based simulation.

Relevance: Validated models will be used to inform the design and operation of RRB's process and will be communicated to industry for broad application, thus supporting BETO's goals for the commercialization of advanced drop-in jet and diesel fuels by 2020.

Image credit: Jenike and Johanson

Key Milestones



Go/No-Go June, 2019: (1) **Validate hopper-flow DEM model** with experimental data from test-scale hopper. (2) **Validate screw-feeder CFD model** with experimental data from pilot-scale screw feeder. (3) **Demonstrate particle-scale pyrolysis models** provide accurate predictions.

Project Budget Table

	Original Project Cost (Estimated)			Project Spending and Balance		Final Project Costs
Budget Periods	**DOE Funding**	**Project Team Cost Shared Funding**	**Contingency**	**Spending to Date**	**Remaining Balance**	**What funding is needed to complete the project.**
Total	$1,800K	$452K		$613	$1,639K	$1,639K
Task 1	$600K	$151K		$204K	$546K	$546K
Task 2	$600K	$151K		$204K	$546K	$546K
Task 3	$600K	$151K		$204K	$546K	$546K

Quad Chart Overview

Timeline

- Start: January 1, 2018
- End: December 31, 2020
- 33% complete of review cycle

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded			$324K	$1,476K
Project Cost Share (In-kind, Total)			$90K	$361K
Red Rock Biofuels, in-kind			$24K	$96K
Jenike & Johanson, in-kind			$30K	$120K
Valmet, in-kind			$15K	$60K
U. Toledo, in-kind			$21K	$85K

Barriers addressed

- Ft-H. Biomass Material Handling and Transportation
- Ct-B. Efficient Preprocessing and Pretreatment
- Ct-F. Increasing the Yield from Catalytic Processes

Partners and collaborators

- Partners
  - NREL (44%)
  - Red Rock Biofuels (12%)
  - Jenike & Johanson (20%)
  - Valmet (10%)
  - U. Toledo (14%)
- Collaboration with FCIC, CCPC, and Purdue’s IBRO project

Objective:

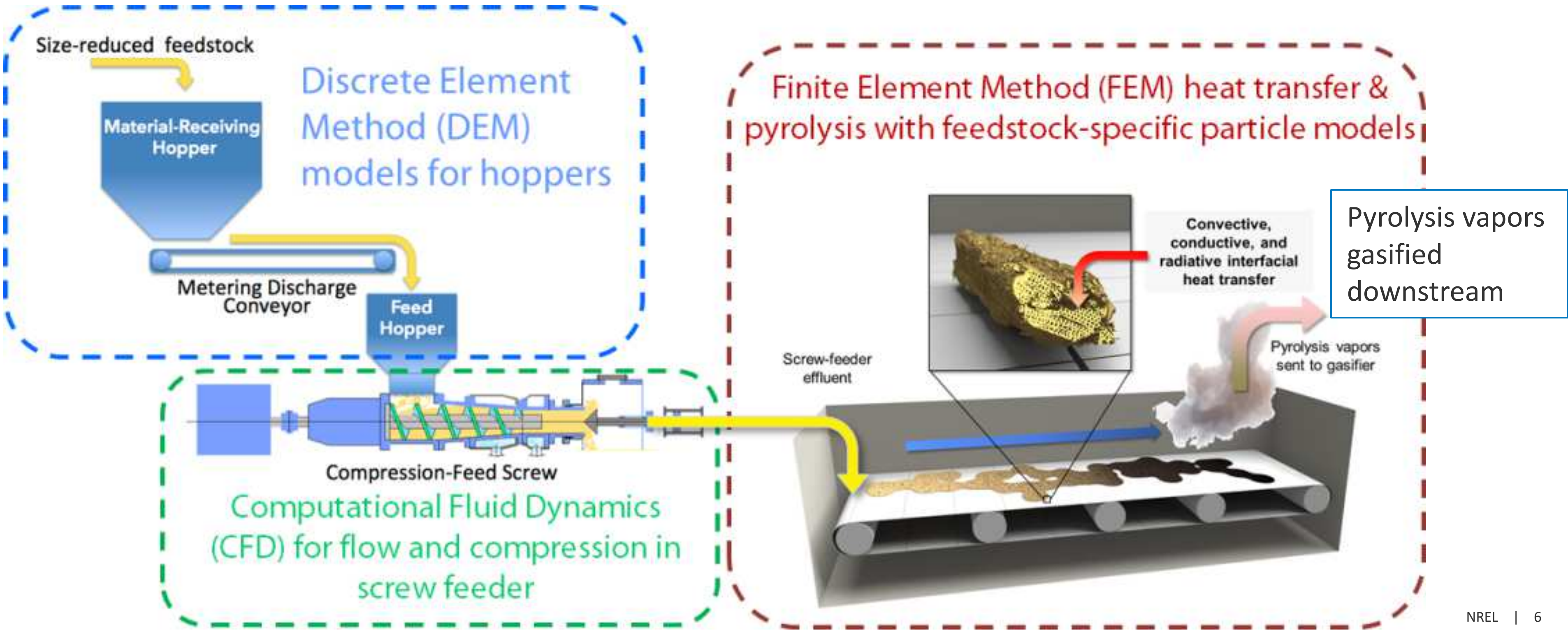
Develop robust physics-based models for the feed-handling unit operations at the front end of the Red Rock Biofuels’ (RRB) gasification process.

End of Project Goal:

Optimized and reduced-risk deployment of an industrial biomass gasification process enabled by high-fidelity physics-based simulation.

Project Overview

- Develop integrated simulations for feed handling and reactor feeding systems, in general, and for Red Rock Biofuels' gasification process, specifically
- Leverage BETO-funded projects in CCPC and FCIC
- Multi-institution team: NREL, Red Rock Biofuels, U. Toledo, Jenike & Johanson, and Valmet
- Funded via DE-FOA-0001689 (Integrated Biorefinery Optimization)
- 3-year project started January, 2018

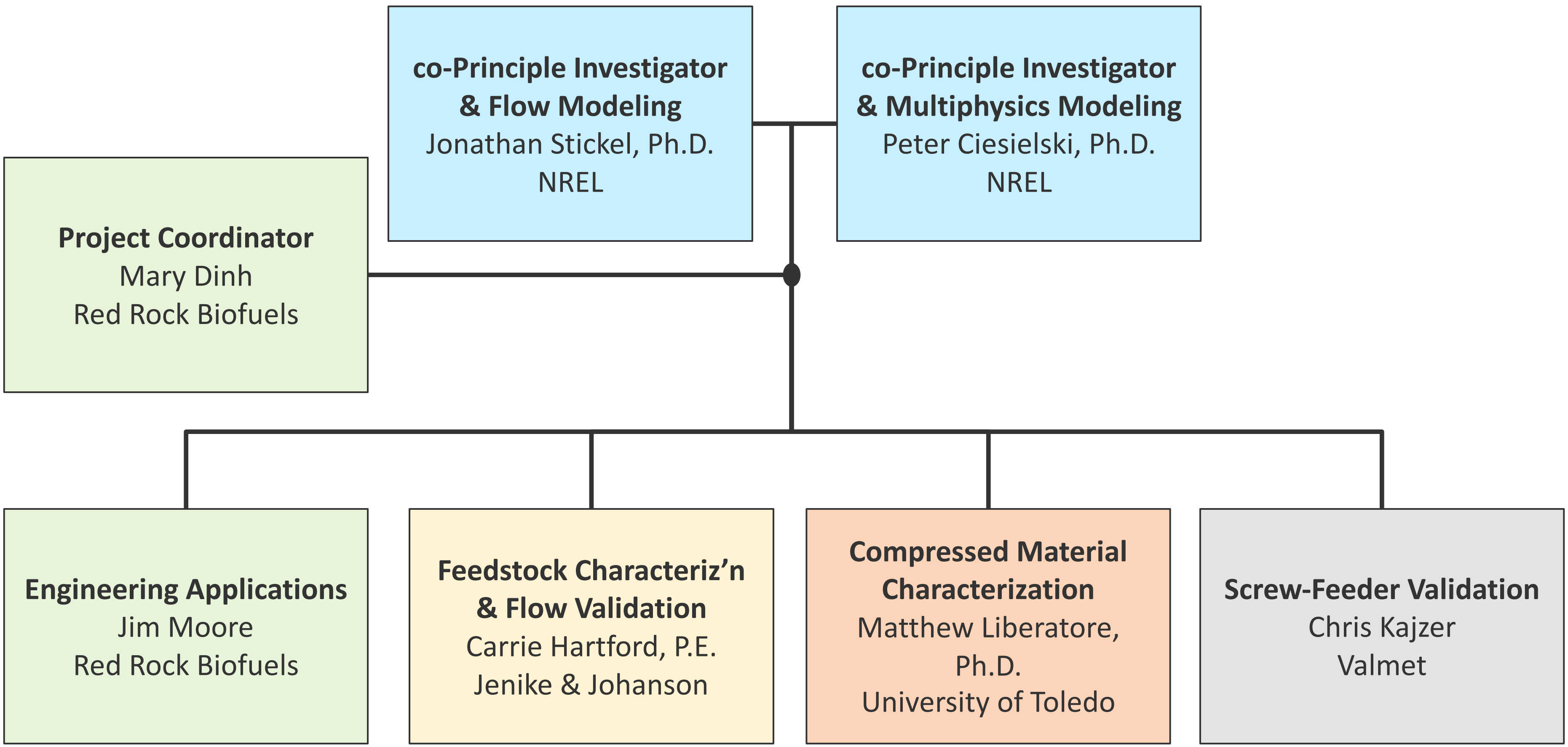


Critical Success Factors and Challenges

Project Component	Critical Success Factor	Challenges/Risks	Approach/ Mitigation strategy
DEM modeling of hopper	Simulations capture behavior of complex, variable feedstock	Very large number of particles required; spheres are poor approximation	Massively parallel computing; develop new code to allow for new particle geometries (glued spheres)
CFD modeling of compression screw-feeder	Simulations can predict failure scenarios as a function of operating conditions and feedstock parameters	The CFD software package is not capable of performing realistic simulations of biomass flow for reasonable computational times	Challenge CFD software ASAP to determine whether qualitative results are correct; switch CFD software if necessary
Multiphysics modeling of biomass pyrolysis	Prediction of optimal conversion conditions and expected yields of RRB's feedstock	Feedstock parameters exhibit large variability; unique reactor design not previously modeled	Generalize models and utilize ensemble calculations; work with reactor designer to understand/predict performance.

Approach - Management

- Overall scientific direction by co-PIs Stickel and Ciesielski
- Technology area leads direct specific project tasks
- Team meetings monthly by conference call and yearly in person
- Subcontracts in place with all team members (FY18 deliverable)

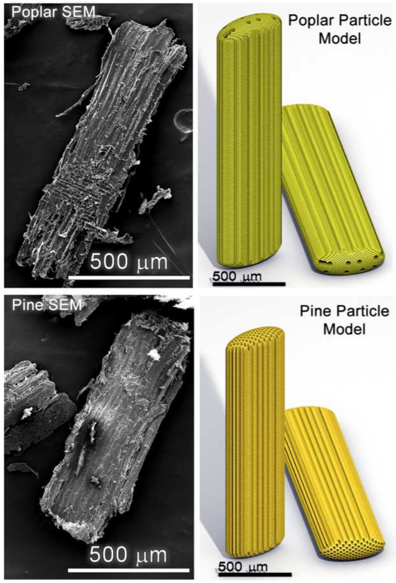


Approach – Team (Continued…)

National Renewable Energy Laboratory (NREL), Lead Institution:

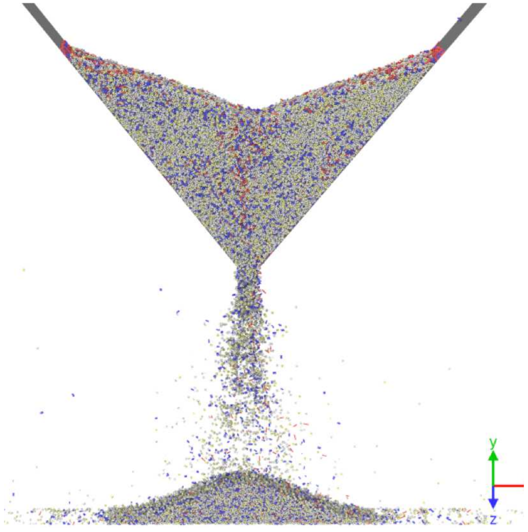
- Jonathan Stickel and Peter Ciesielski, co-PIs
- Directing the project and leading modeling work
- Leveraging previous and ongoing modeling work in Consortium for Computational Chemistry and Physics (CCPC) and Feedstock Conversion Interface Consortium (FCIC).

State-of-the-art biomass particle models developed previously by the CCPC



Ciesielski, et al. Energy & Fuels, 2015
Pecha et al. ACS Sust. Chem. Eng., 2017

Feedstock flow models are being developed in the FCIC



CCPC

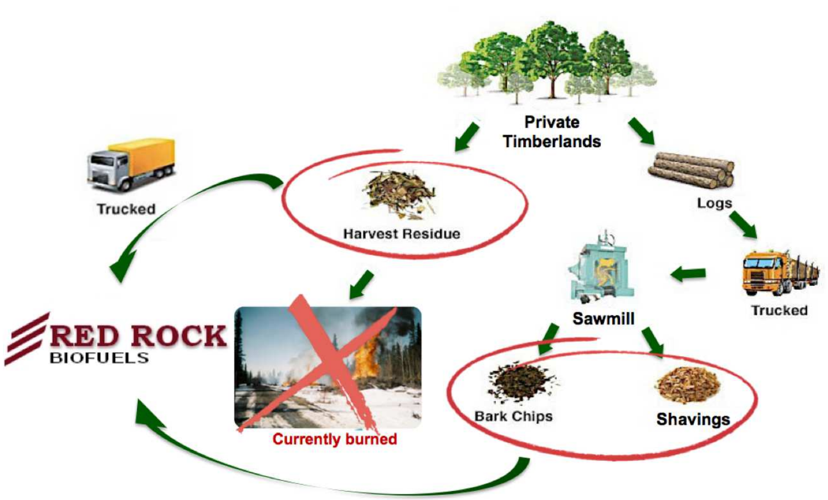
fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Approach – Team (Continued…)

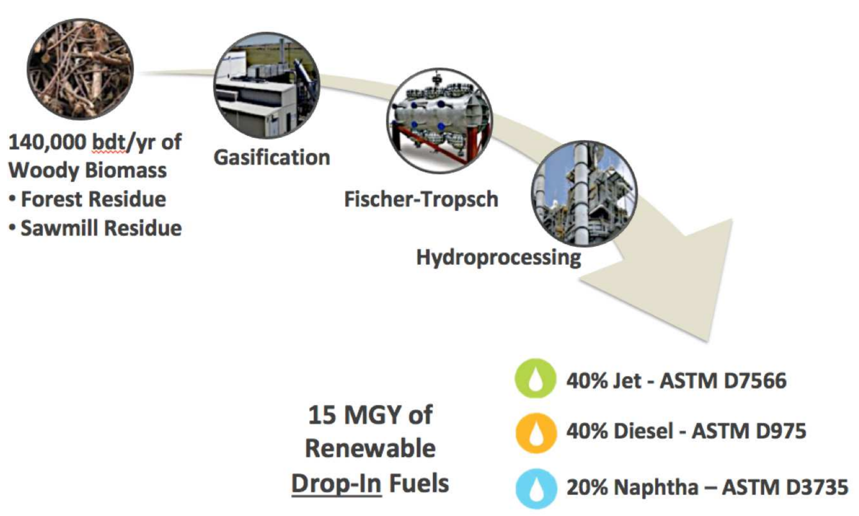
Red Rock Biofuels (RRB):

- Mary Dinh and Jim Moore
- Developing commercial-scale biorefinery using gasification and Fischer-Tropsch conversion process
- RRB's feedstock and process are to be target application of modeling work

Target Feedstock



First Commercial Project – Lakeview, OR



Approach – Team (Continued…)

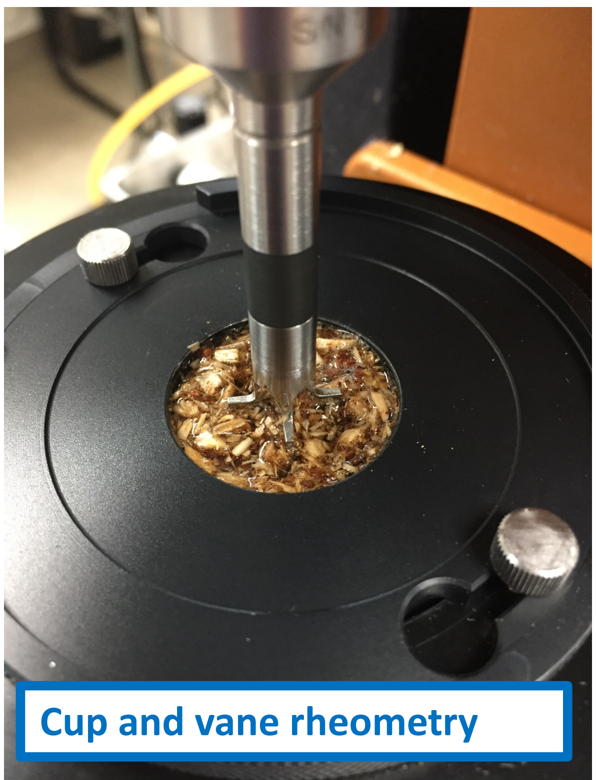
Jenike and Johanson (J&J):

- Carrie Hartford and David Craig
- Leader in bulk material handling
- Performing bulk material property measurement of feedstocks and hopper-flow validation

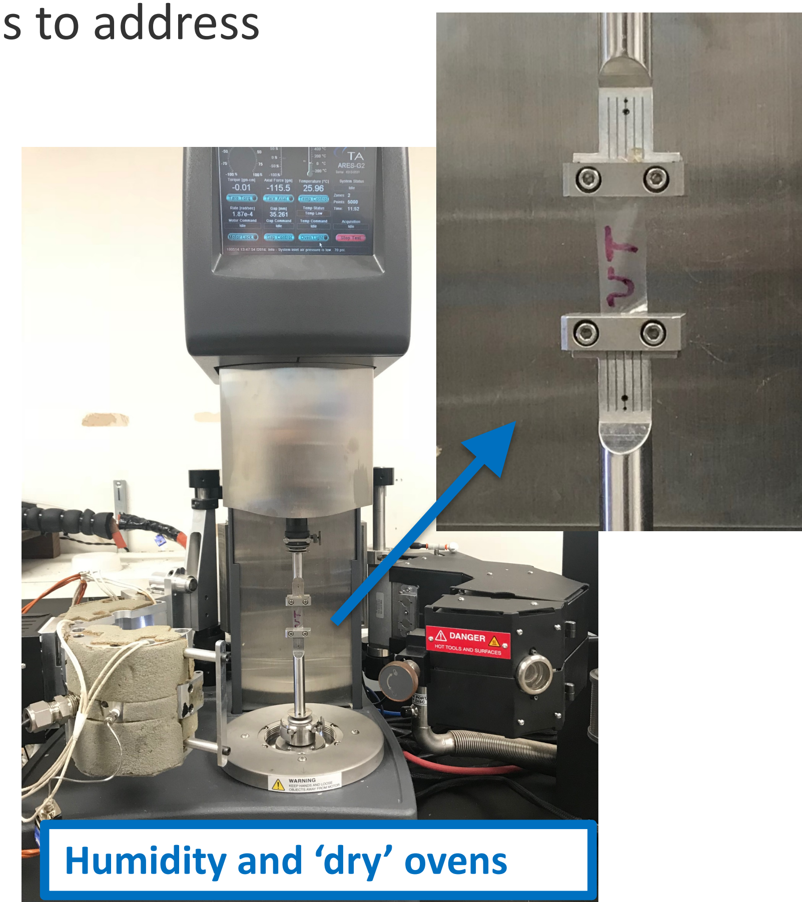
Approach – Team (Continued…)

University of Toledo:

- Professor Matthew Liberatore and graduate students
- Rheology and fluid mechanics expert
- Measuring the rheology of compressed biomass
- Implementing multi-faceted approaches to address ‘difficult’ materials



Cup and vane rheometry

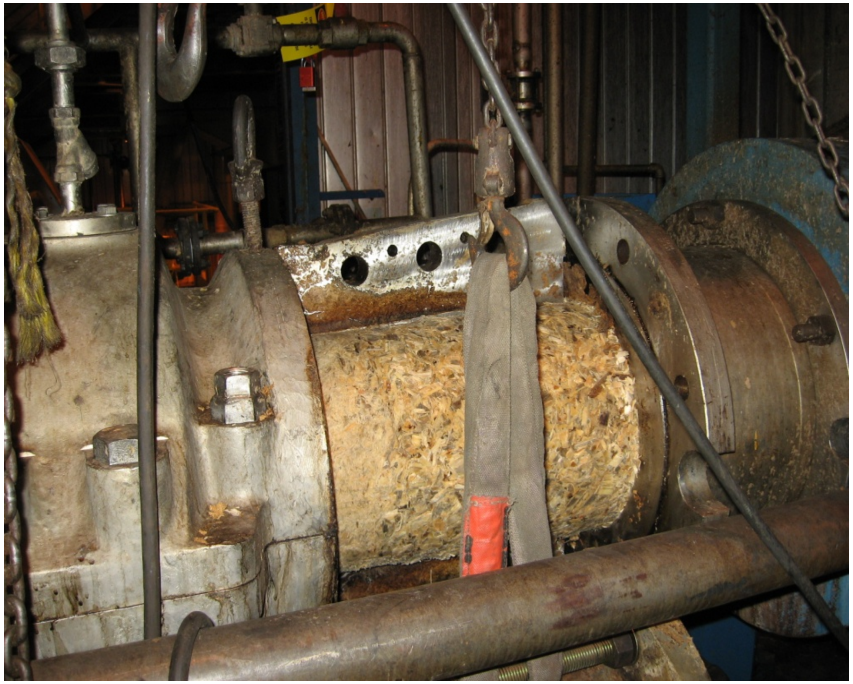


Humidity and ‘dry’ ovens

Approach – Team (Continued…)

Valmet:

- Chris Kajzer and Garth Russell
- Extensive experience in design and operation of compression-screw feeders (about 70 years of experience in pulping, fiberboard and high pressure feeding and sealing)
- Supporting development of compression-screw feeder model and validation

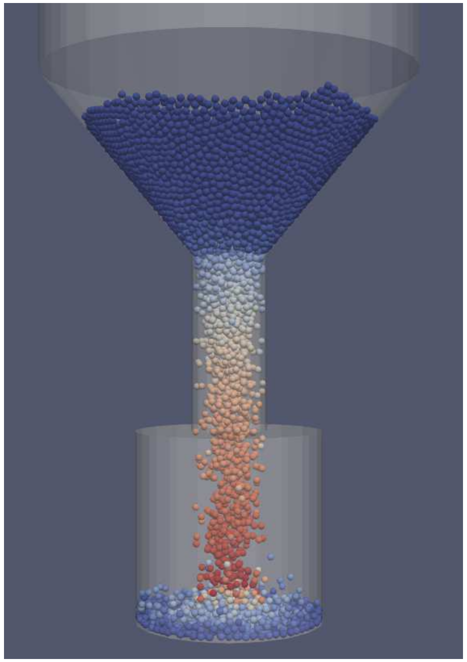


Task 1: Hopper Modeling (approach)

Current state-of-the-art for modeling dense flow of granular media is the discrete element method (DEM)

- Forces and motion of each individual particle is accounted for
- Elastic spherical particles: large systems
- Elastic non-spherical models in commercial codes: small systems
- No codes have reproduced flow of biomass particles at process scales
- Massively parallel simulations are performed on NREL's HPC systems (Peregrine and Eagle)

Image credit: Jenike and Johanson

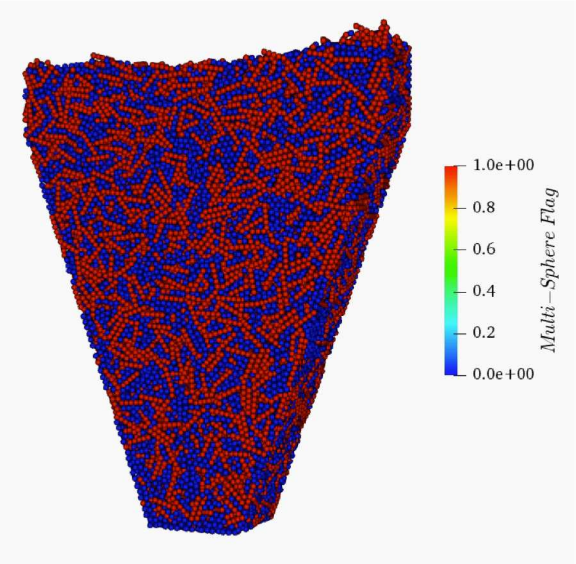


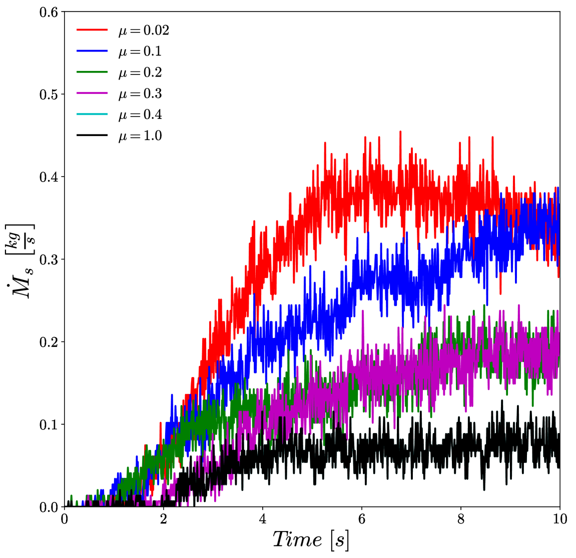
Bulk material measurement

- Compressibility
- Permeability
- Cohesion
- Wall friction
- Chute tests

Validation via dedicated hopper tests (arching, flow rate)

Task 1: Hopper Modeling (progress)





Work to date:

- Evaluated DEM contact models
- Implemented and compared novel methods
  - Inhibited rolling with spherical particles
  - Rods composed of glued-spheres
- Dynamic simulation with 10^6 particles
- Tuned parameters to represent bulk biomass behavior

Future Work:

- (FY19) Further develop, parameterize, and validate DEM model to accurately represent flows of woodchips in hoppers.
- (FY20) Use DEM model to evaluate flow performance in material-receiving hopper of size ~100 m^3 (~10^8 particles to be simulated).

Task 2: Screw-feeder Modeling (approach)

Computational fluid dynamics (CFD) to model the compressed and deforming biomass material

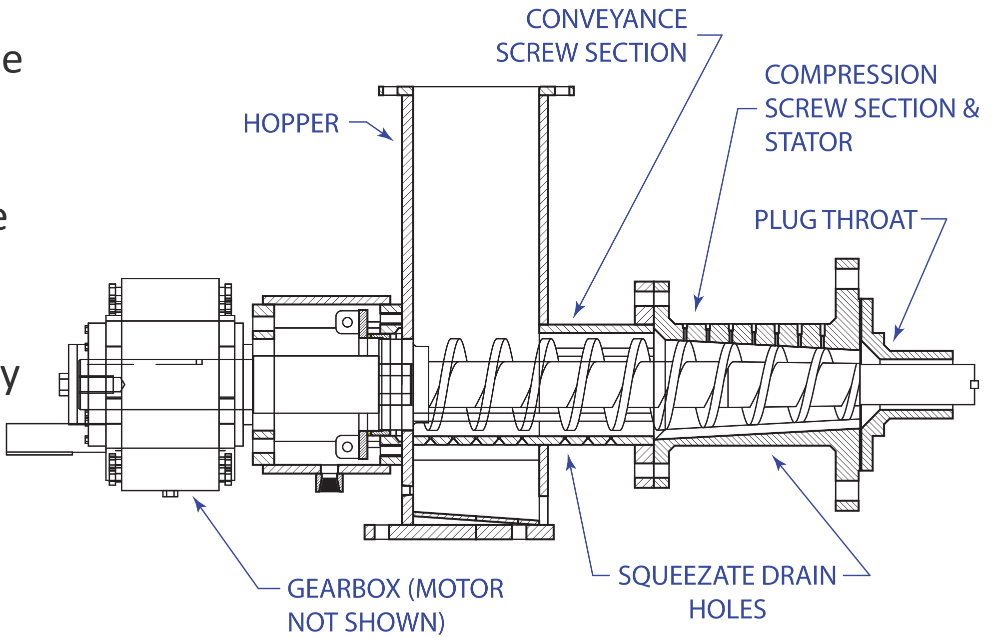
- High pressure (up to 300 psi) and pressure gradients compress the biomass into a single material
- Will implement a 3-phase compressible mixture model with non-Newtonian rheology

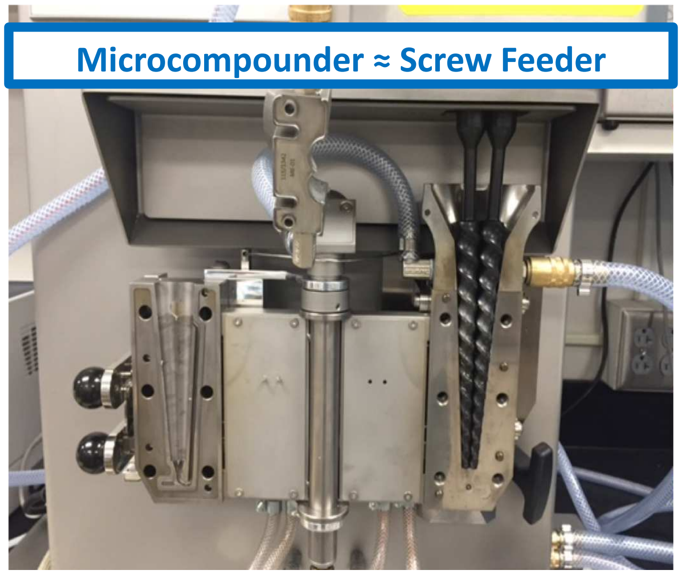
Material measurement:

- Benchtop twin-screw extruder (microcompounder) to measure material response under compression

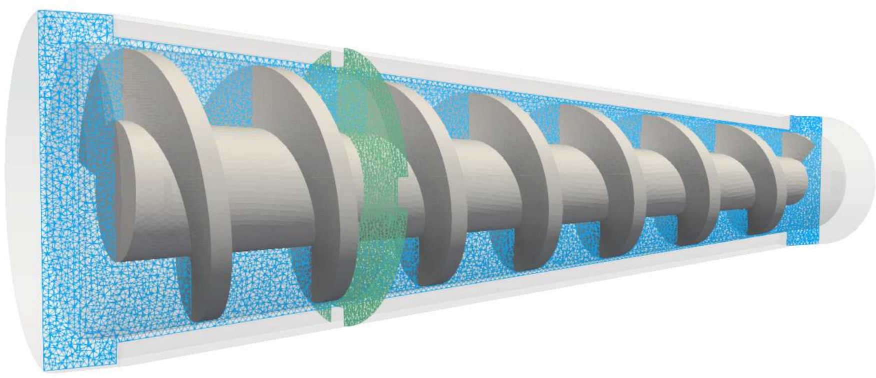
Validation:

- The CFD of compressed biomass through plug screw feeders will be validated against experimental data in plug screw feeders
  - 4” plug screw feeder at NREL
  - Valmet will also supply validation data either by historical data mining or by experiment for commercial scale plug screw feeders of at least 5” in diameter.



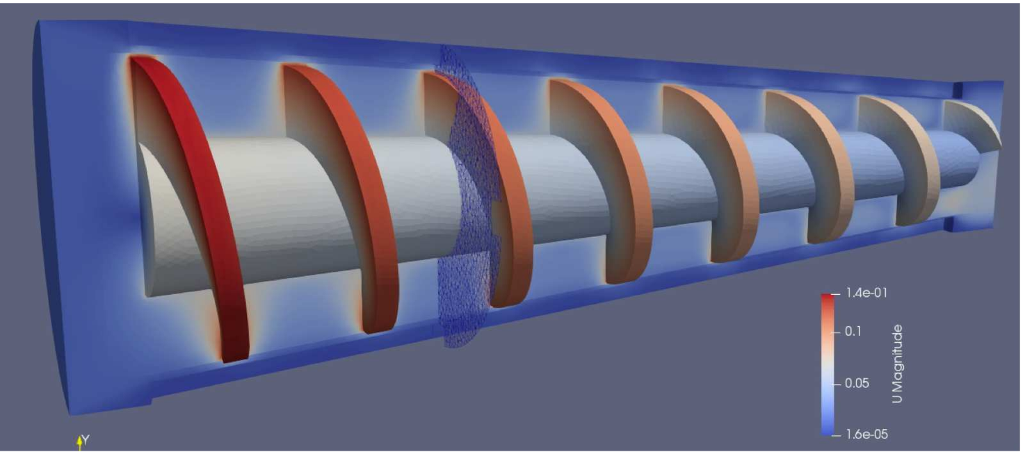


Task 2: Screw-feeder Modeling (progress)



Work to date:

- Model development co-funded with 1.1.2.502 (FCIC)
- Defined computational mesh for compression zone:
  - Rotating screw region and non-rotating stator region
  - ~10^6 cells
- Bingham yield-stress viscosity model with parameters inferred from literature
- Preliminary simulations of 10 s took 48 h on 128 cpus
- Evaluated wall shear stress on the auger surface



Future Work:

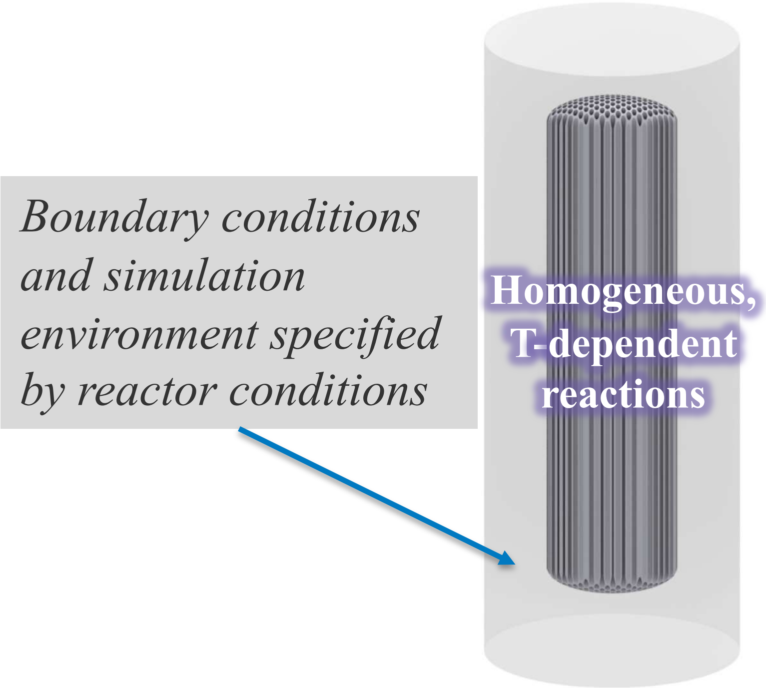
- (FY19) Implement density-dependent viscosity model in CFD and perform experimental validation.
- (FY20) Use CFD model to evaluate flow performance reduce operational risk of industrial compression-screw feeder.

Task 3: Pyrolyzer Modeling (approach)

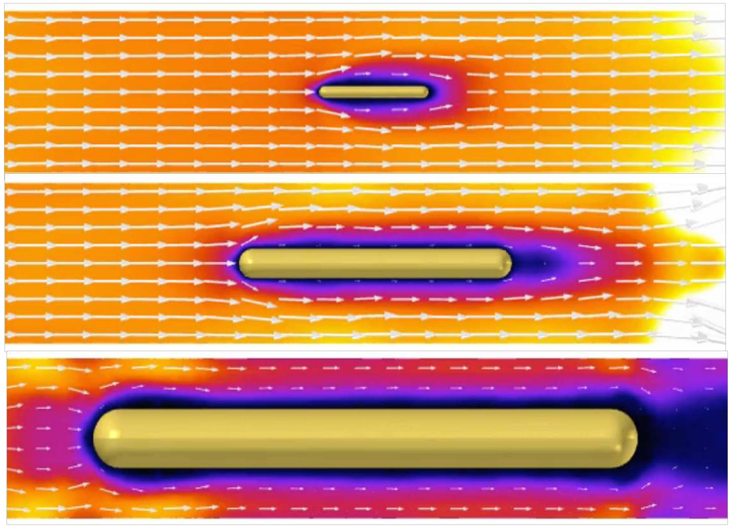
- **Multiphysics modeling** of heat and mass transfer coupled to thermochemical conversion reactions for individual particles that span the range of sizes, shapes, and species present in the feedstocks
- **Ensemble calculations** that account for the heterogeneous particle and residence time distributions to estimate yields, optimal residence times, and corresponding operating conditions (e.g., conveyor speed)

Validation will be performed by two methods:

- **Lab-scale pyrolysis experiments** using RRB's feedstock in a horizontal flow reactor at NREL
  - Can approximate reactor environment delivered by the full-scale conveyor/pyrolyzer unit by modulating the flow rate and temperature
  - Coupled to MBMS analytical system to determine detailed speciation of pyrolysis products to assess quality (not just yield)
- **Full scale conveyor/pyrolyzer runs** performed by RRB
  - Will verify that simulation results are representative of industrially-relevant process scales



Task 3: Pyrolysis Modeling (Progress)



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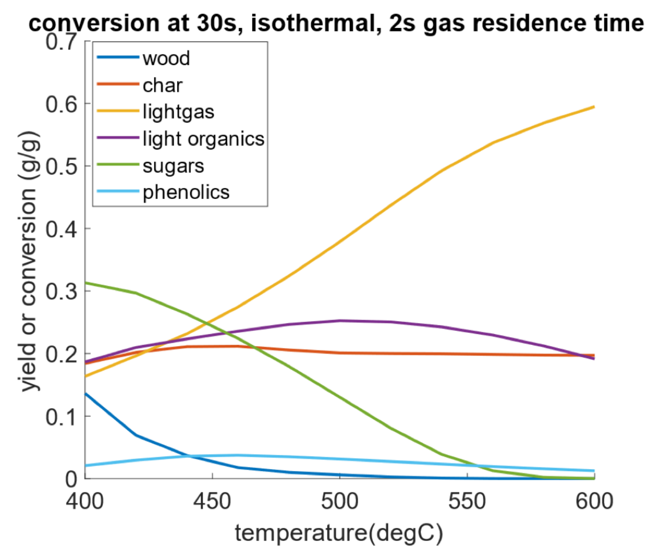


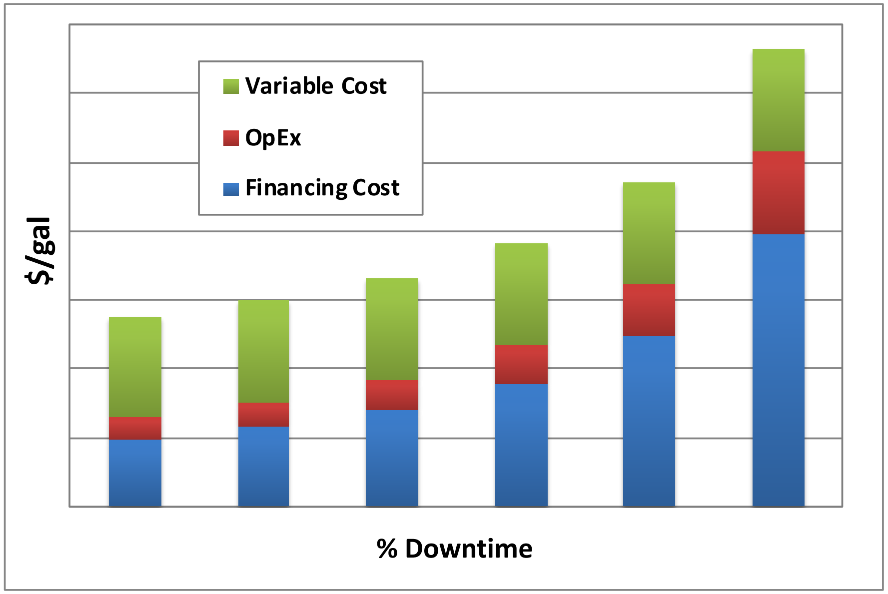
- Feedstock characterization results were used to construct pyrolysis simulations for feedstock particles that capture the range of size, shape, and moisture content of the RRB feedstock.
- Ensemble calculations are used to estimate optimal residence times (controlled by the conveyer speed) as a function of feedstock attributes.
- Parametric sweeps are used to investigate in-silico the impact of varying reactor operating conditions.
- **Provided technical reports to RRB summarizing conditions for optimal conversion of RRB's feedstock.**

Future Work: Complete lab and commercial-scale experiments for initial validation. Use validated simulations to perform sensitivity analysis over feedstock attributes and provide guidance to RRB

Relevance

The **validated transport and reaction models** developed in this project will:

- Inform the design and operation of RRB's process
- Identify and quantify potential risks and associated with the RRB process and suggest mitigation strategies, thus leading to **minimal production downtime**
- Provide rigorous, science-based guidance to biorefinery and bioproducts industry during initial process design phase
- Allow for computational screening of probable operation scenarios
  - Improve fidelity of TEA
  - **Reduced risk for investors**
- Ultimately, supports BETO's goals for commercialization of advanced drop-in jet and diesel fuels by 2020 (2016 MYPP)



Effect of downtime on RRB's total cost per gallon

Relevance (continued)

Communication and Market Impacts

- Modeling and simulation:
  - The modeling and simulation tools, with general-use findings, will be published in 3-6 peer-reviewed manuscripts (1-2 per task)
  - Modeling code base will be stored and managed at NREL; it will be made available upon request and as part of partnership agreements
  - Frequent communication and collaboration with FCIC and CCPC consortiums
- Red Rock Biofuels:
  - Secured financing
  - Broke ground for a production facility in Lakeview, Oregon.
  - Secured contracts for produced jet and diesel fuels

Our collaboration with NREL and the project team has provided valuable insights regarding the complexities of biomass feedstocks that have helped inform the design process for our first commercial project. Additionally, the project with NREL is developing computational tools that will help us adapt and optimize our operational processes for new feedstocks and de-risk future projects. -- Red Rock Biofuels Management

Image: https://www.redrockbio.com/technology.html

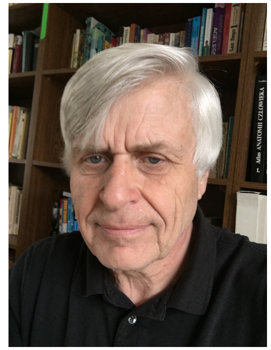
Summary

- **Overview**: Physics-based computational modeling to address front-end feeding and reaction of an industrial biorefinery; these unit operations have experienced high failure rates in previous biorefinery startups.
- **Approach**: High-impact team capable of executing the various parts of the project.

  Computational model and simulations supported by state-of-the-art material measurements and unit-operation experiments.
- **Results**: Work progress is on track and meeting planned deliverables.

  Technical modeling results have already influenced the design and planned operation of RRB equipment.
- **Future Work**: Verify models against experiments and use simulations to inform design and operation
- **Relevance**: Validated models will be used to inform the design and operation of RRB's process and will be communicated to industry for broad application, thus supporting BETO's goals for the commercialization of advanced drop-in jet and diesel fuels by 2020.

Jonathan Stickel, Peter Ciesielski (NREL)



Chris Kajzer (Valmet)

Mary Dinh, Jim Moore (RRB)

Cary Hartford (J&J)

Matt Liberatore (U Toledo)

U.S. DEPARTMENT OF ENERGY

Thank You

www.nrel.gov

Jonathan.Stickel@NREL.gov

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Publications

- Aaron M. Lattanzi and Jonathan J. Stickel. “Hopper Flows of Spherical and Rod-Like Particles via the Multi-Sphere Method.” *In Preparation*.
- M. Brennan Pecha, Jorge Ivan Montoya, Manuel Garcia-Perez, Farid Chejne, and Peter N. Ciesielski. “Key intra-particle phenomena of lingocellulosic materials pyrolysis: Chemical reactions, heat transfer, mass transfer, and phase change.” *In Preparation.*

Presentations

- Rahimi M., Sitaraman H., Lischeske J., Sievers D., Kuhn E., and Stickel J. Computational Fluid Dynamics Simulation of Lignocellulosic Biomass Transport in a Compression-Screw Feeder. Poster presentation at the AIChE Annual Meeting, Pittsburgh, PA, October, 2018.

Project Scope Change Table

Scope Changes	Date	Logic / Reasoning	Approval / Rejection Date
No scope changes to date			

Risk Table

Risk	Probability	Mitigation Strategy
The integrated RRB unit operations may not be available for model validation within the timeline of the proposal due to the preliminary startup date	High	We have identified alternative experimental validation strategies for each proposed system based on the existing resources provided by NREL and our industrial partners. Models for the hopper systems may be validated with similar units owned by J&J. Models for the plug screw feeder may be validated with similar units owned by NREL and/or Valmet, and historical operational data provided by these institutions. Models for feedstock pyrolysis will be validated using data provided by TCG Global's demonstration scale (10 dtpd) conveyer/pyrolyzer unit.
The proposed DEM and CFD software packages are not capable of performing physically realistic simulations of biomass flow for reasonable computational times (<2 weeks per simulation).	Low	We will start developing flow models and performing simulations as soon as possible to verify that expected qualitative flow behaviors can be achieved using the preferred software. If the preferred software is not able to perform satisfactorily, we will switch to other, possibly commercial, software packages early in the project timeline, adjusting resources as necessary.
Lab-scale validation experiments are not reflective of conditions delivered by the RRB conveyor/pyrolyzer	Moderate	Uncertainties will be quantified by performing parameter sweeps to consider a range of scenarios by which conditions could differ between the 2 systems. These are described in greater detail in Milestone 3.7 in the proposal.

Risk Table (continued)

Risk	Probability	Mitigation Strategy
Feedstock properties are inconsistent with characterization data provided by supplier; Feedstock properties may vary year-to-year	Moderate	We plan to perform in-house characterization of the feedstock properties, including size and shape distributions, surface roughness, moisture content, air content, compressibility, thermal conductivity, heat capacity, viscosity, elastic modulus, and yield stress. Simulations will first be developed and parameterized for the real RRB feedstock; then hypothetical feedstocks with a range of properties will be simulated to provide RRB with guidance regarding how to adjust process conditions to accommodate variations in feedstock properties.
Models are unable to predict results of validation experiments within an acceptable tolerance	Low	We have planned 3 Go/No-Go decision points over the course of the project at which model efficacy will be evaluated. Decisions for continuation of the modeling efforts will be contingent upon the agreement of the simulation predictions with experimentally obtained validation data. In the unlikely case that predictive models are not achievable with present computational methods or resources, projects will be discontinued and financial resources redistributed or returned to BETO.