Integrated Computational Tools to Optimize and De-Risk Feedstock Handling & High-Pressure Reactor Feeding Systems: Application to Red Rock Biofuels' Biorefinery (WBS 3.1.1.001/3.3.1.2)

March 23, 2021

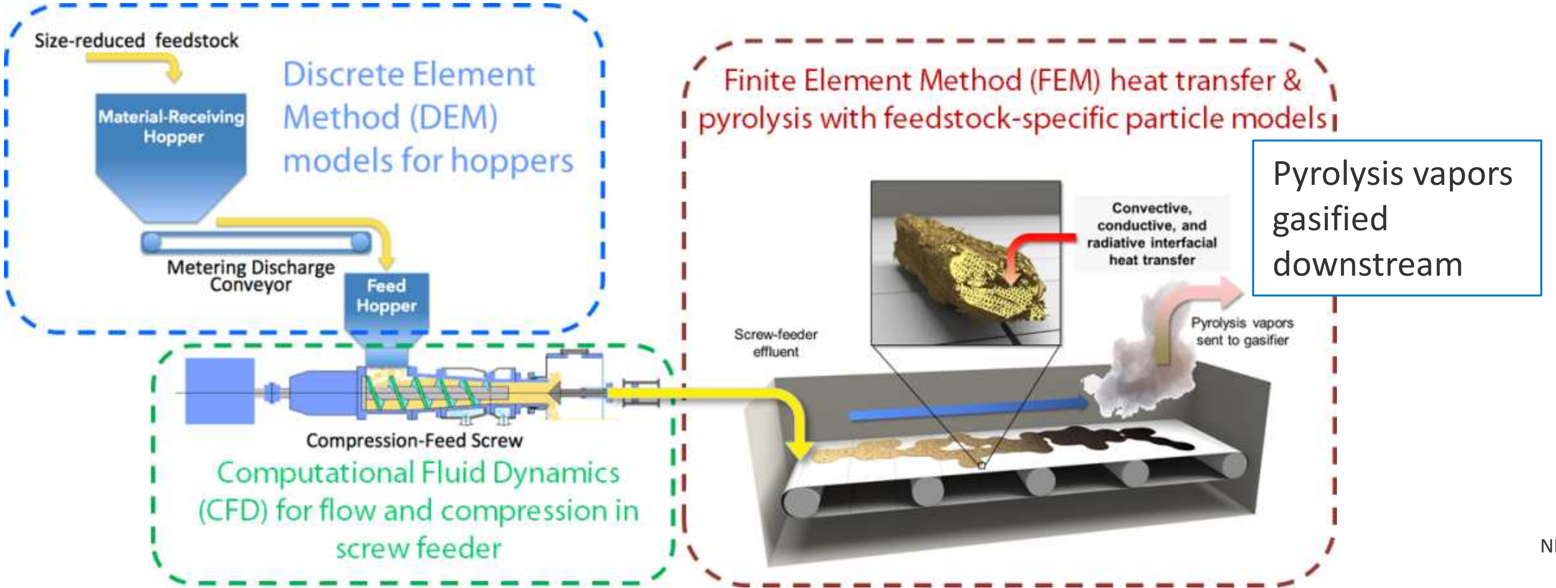
Systems Development and Integration

Jonathan Stickel (*presenter*) and Peter Ciesielski

National Renewable Energy Laboratory

Project Overview

- Objective: **optimize** and **de-risk** the deployment of biomass gasification processes by implementing **physics-based simulations** of feed handling and transportation unit operations
- Modeling and simulations supported **Red Rock Biofuels** (RRB) during design and build of their commercial facility
- Physics-based models provide high-confidence approach for **design and scale-up** of process technology (compared to empirical or basic-engineering approaches)
- Funded via DE-FOA-0001689 (Integrated Biorefinery Optimization).
- January 2018 – June 2021



Market Trends

Product

- Anticipated decrease in gasoline/ethanol demand; diesel demand steady
- Increasing demand for aviation and marine fuel
- Demand for higher-performance products
- Increasing demand for renewable/recyclable materials

Feedstock

- Sustained low oil prices
- Decreasing cost of renewable electricity
- Sustainable waste management
- Expanding availability of green H_2
- Closing the carbon cycle

Capital

- Risk of greenfield investments
- Challenges and costs of biorefinery start-up
- Availability of depreciated and underutilized capital equipment

Social Responsibility

- Carbon intensity reduction
- Access to clean air and water
- Environmental equity

NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Value Proposition

- **Optimize and de-risk deployment** of an industrial biomass gasification process enabled by high-fidelity physics-based simulation

Key Differentiators

- Physics-based models at multiple scales are used to properly represent complex biomass behaviors
- Multi-institution team capable of material characterization, modeling, and validation

Management, Team Overview

- Overall scientific direction by co-PIs Stickel and Ciesielski
- Technology area leads direct specific project tasks

- Regular team meetings coordinated modeling and experimental work as well as engineering applications

co-Principle Investigator & Flow Modeling
Jonathan Stickel, Ph.D.
NREL

co-Principle Investigator & Multiphysics Modeling
Peter Ciesielski, Ph.D.
NREL

Project Coordinator
Mary Dinh
Red Rock Biofuels

Engineering Applications
Jim Moore
Red Rock Biofuels

Feedstock Characteriz’n & Flow Validation
Carrie Hartford, P.E.
Jenike & Johanson

Compressed Material Characterization
Matthew Liberatore, Ph.D.
University of Toledo

Screw-Feeder Validation
Chris Kajzer
Valmet

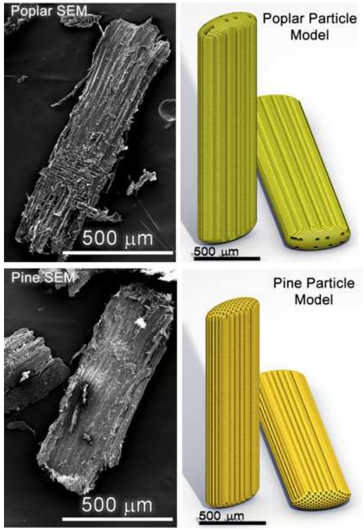
National Renewable Energy Laboratory (NREL), Lead

- 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).

Jonathan Stickel

Peter Ciesielski

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

Chipped loblolly pine particles | **Polyhedral particles of arbitrary shapes** | **A v-shape hopper discharge simulation**

Xia, et al. ACS Sustainable Chem. Eng., 2020
Jin, et al. ACS Sustainable Chem. Eng., 2020

CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

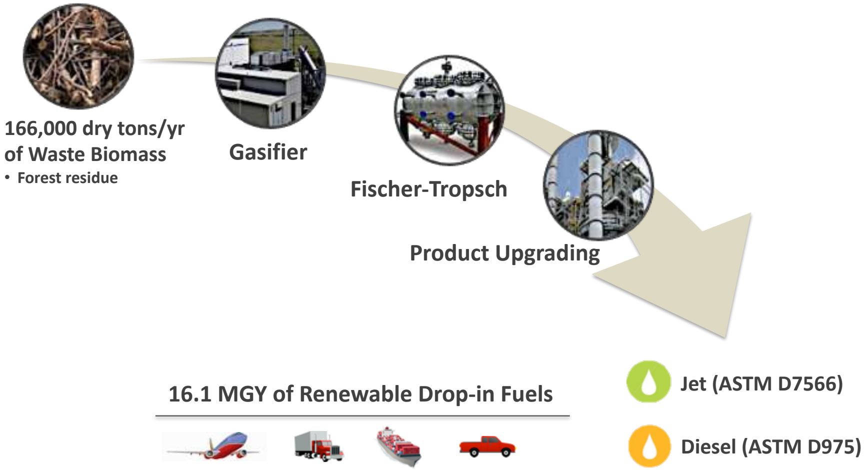
Red Rock Biofuels (RRB)


Mary Dinh


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

First Commercial Project – Lakeview, OR



Jenike & Johanson


Carrie Hartford

- Leader in bulk material handling
- Performing bulk material property measurement of feedstocks and hopper-flow validation

University of Toledo

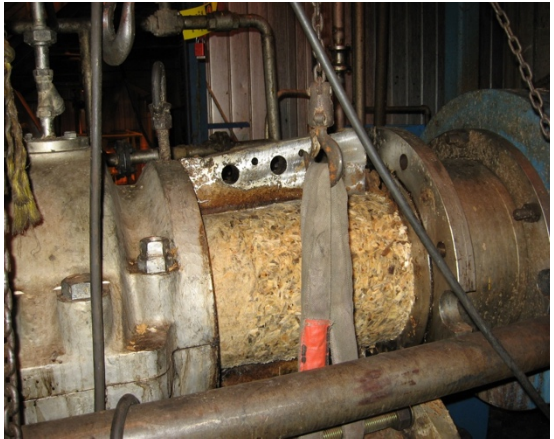
Matt Liberatore

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

Valmet

Chris Kajzer

- 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



Risk Mitigation and Project Changes

Project Component	Challenge/Risk	Changed Approach	Outcome
DEM modeling of hopper	Very large number of particles required; spheres are poor approximation	Two simulation approaches pursued simultaneously: (1) research-code DEM of ~10^8 spherical particles, (2) vendor code DEM of ~10^6 rod-like particles	*In progress*: Simulation results from both approaches together inform hopper/silo design and operation
CFD modeling of compression screw-feeder	Higher operational speed of commercial-scale feeder caused CFD methods to crash	Identified method for simulation startup that involved incrementing the screw speed	Agreement achieved between measured and simulated torque of commercial-scale feeder
Multiphysics modeling of biomass pyrolysis	Particle-scale models are insufficient to represent mass and heat transport in RRB pyrolysis reactor	Worked closely with RRB to develop reactor-scale model	Reactor-scale simulations are informing RRB of feedstock properties needed to achieve desired conversion

- Project extended from December 2020 to June 2021 in response to overall pace of progress

Technical Approach

Scientific approach:

1. Develop physics-based models
2. Inform model parameters by material characterization
3. Validate models with experimental data, performed in at-scale process equipment where possible
4. Use models to inform optimal design and operation of RRB's process; publish models for use in industry

Three tasks:

1. Hopper & silo discharge
2. Plug-screw feeder operation
3. Pyrolyzer operation

Go/No-go Decision points:

1. Place subcontracts for the team (6/30/18)
2. Experimentally validate models for all tasks by achieving **quantitative agreement within 10%** (9/30/19)
3. Demonstration and/or validations of models (all tasks) **at commercial scale** (9/30/20 & 11/15/20)

Task 1, Hopper & Silo Discharge (*approach*)

Advancing the current state-of-the-art **discrete element method (DEM)** solver to model the biomass feedstock flow in commercial feeding system

- Modeling **irregularly shaped biomass particles** using two approaches:
  - Rod-like particles using **glued-spheres**
  - **Representative spheres** with high rolling resistance
- Develop DEM solver capable of running industry-scale simulations with **10^8 particles** (GPU code, ORNL Summit)

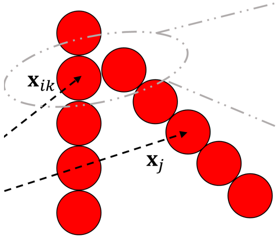
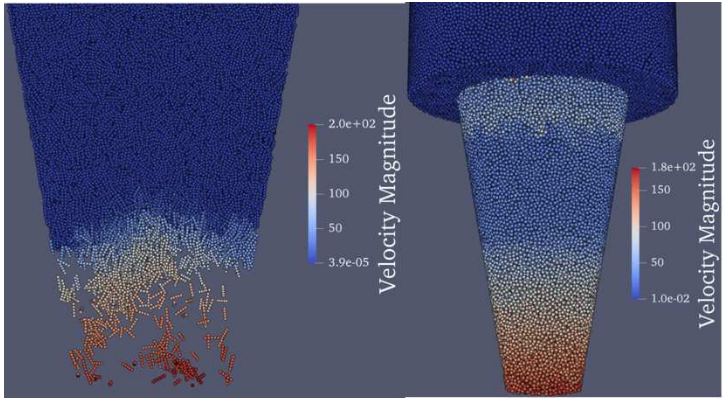


Image credit: Jenike and Johanson

Material measurement and validation

- Compressibility, internal and wall friction, cohesion
- Hopper discharge flow experiments for **validation**
- Identify operating conditions leading to **process upsets**



Conical hopper discharge simulation using glued-sphere (left) model and representative non-rolling sphere (right) model

Task 2, Plug-Screw Feeder Operation *(approach)*

Experimental approach:

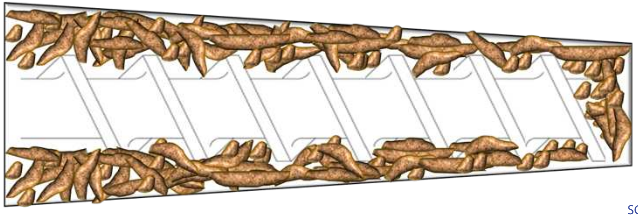
- Benchtop twin-screw extruder (microcompounder) to **measure material flow** under **compression**
- Measured **force** at various screw **speeds** and moisture contents was converted to **viscosity**
- Biomass **compression** data and the **torque** data from a **commercial-scale** screw feeder were acquired

Computational Fluid Dynamics Modeling:

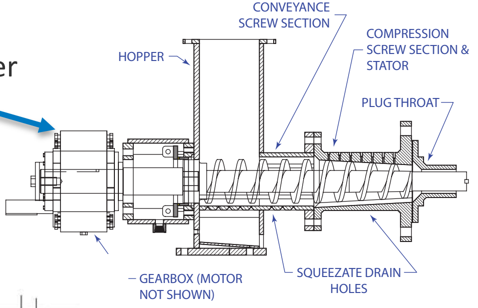
- Develop CFD solver to model biomass in the **compression zone** of screw feeders
- Challenge: **compressible** behavior and **non-Newtonian rheology** of the biomass material under high compression

Validation:

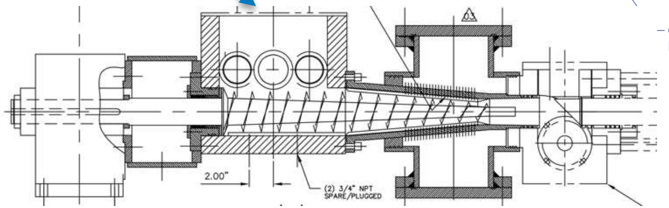
- Experimental measurements of **screw feeder torque** agreed with simulation results
- 2 different screw-feeders, one commercial scale



AB screw feeder



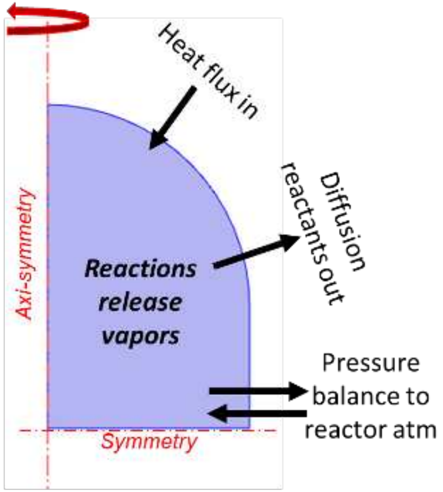
Metso screw feeder



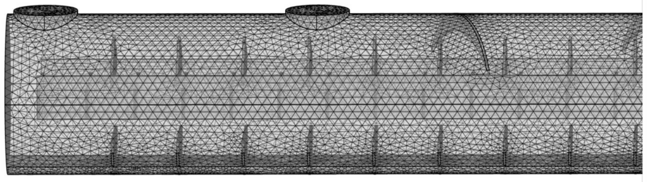
Task 3, High temperature reactor modeling (*approach*)

- Original approach was **particle-scale reaction model** utilizing particle size distributions
- Approach changed to **reactor model** for predicting impacts of material pre-processing and operating conditions on overall **pyrolysis yields**
- Simulations informed by **particle analysis** and **moisture content** measurements of RRB feedstock
- Validation in FY21 with separate follow-on project via FCIC DFO

Particle simulations



Finite Element Method model mesh for RRB reactor



Material Flow

$$\rho_f (u \cdot \nabla) u = \nabla \cdot \left[-p + \mu \left(\nabla u + (\nabla u)^{\mathrm{T}} \right) - \frac{2}{3} \mu (\nabla \cdot u) \mathrm{I} \right]$$

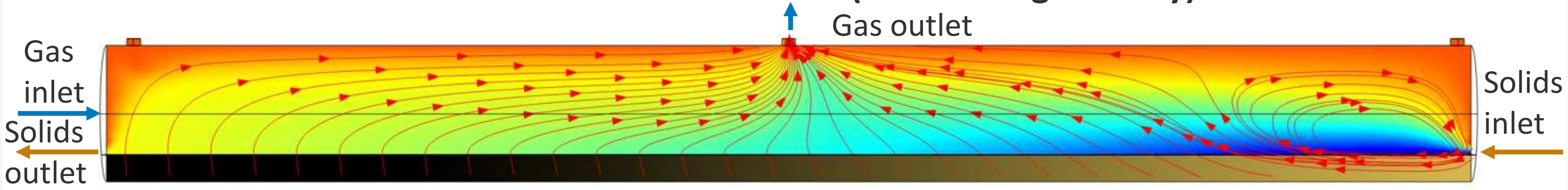
Mixed phase continuum

$$\left(\rho_s C_{P,s} + \rho_f C_{P,f} \right) \langle u \rangle \cdot \nabla T - \nabla \cdot \langle k \rangle \nabla T = Q$$

Heat transfer

$$\rho C_p u \cdot \nabla T - \nabla \cdot k \nabla T = Q$$

Fluid flow and wood conversion with reactor model (not actual geometry)



Impact

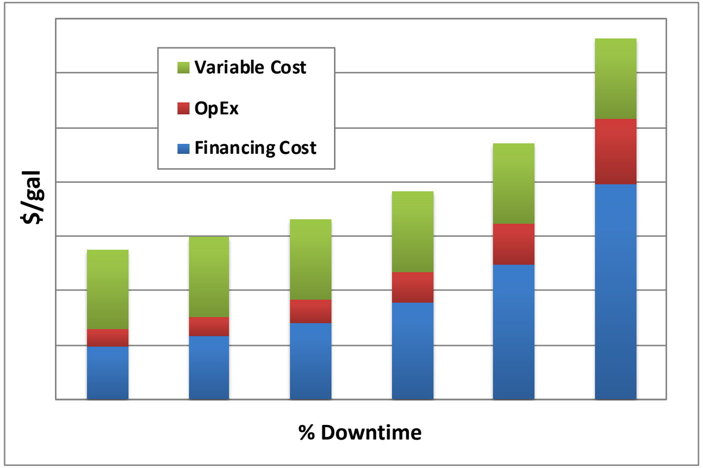
*A high-fidelity, experimentally **validated simulation toolset** for the RRB process front-end to **de-risk, troubleshoot, and optimize***

Validated transport and reaction modeling toolset:

- Provided rigorous, science-based guidance to RRB during design and build of their commercial facility
- Simulation methods to be released as open-source software (github)
- Publications in scientific literature

Flow models:

- State-of-the-art computational models for industrial-scale silos and compression-screw feeders
  - Pushing the envelope of what's possible using HPC hardware
- Confirmed that current designs for RRB process are functional
- Currently being used to probe failure modes and identify reliable operating windows (feedstock properties, flow rates, etc.)

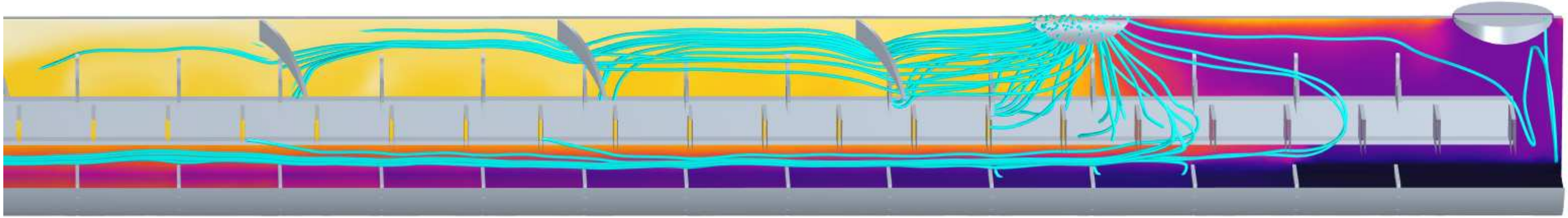


Effect of downtime on RRB's total cost per gallon

Impact, cont'd

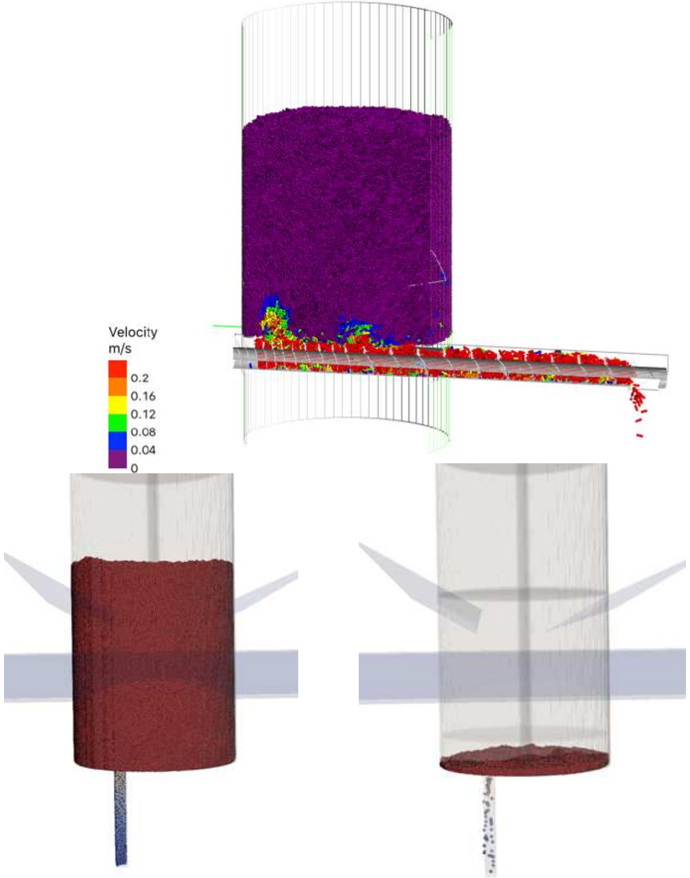
Pyrolysis reactor modeling:

- Identified optimal feed rates and predicted yields as a function of feedstock characteristics including density and moisture content
- Analyzed risks associated with potential heat-transfer bottlenecks; suggested and modeled risk-mitigation strategies



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

Task 1, Hopper & Silo Discharge (*progress/outcomes*)



Commercial scale material receiving bin flow simulation

Outcomes:

- Implemented experimentally validated novel contact models for nonspherical biomass particles
  - Glued-spheres model to represent rod-like chips
  - Non-rolling spherical model
- Developed new hybrid parallel in-house DEM code capable of utilizing GPUs on state-of-the-art HPC system
- Performed flow simulation of 47 million particles in industry-scale material-receiving silo (V ~ 100 m^3)
- Performed simulation of material-receiving hopper flow with internal moving components (Jenike in-house code)

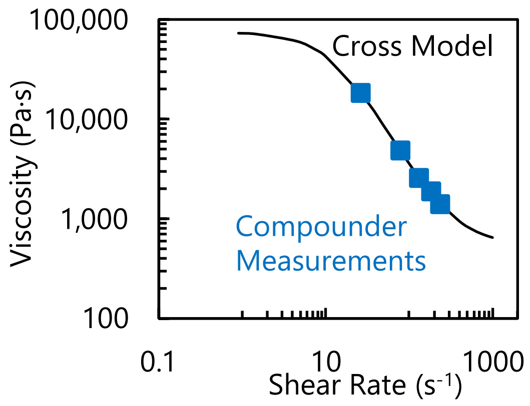
Remaining Work:

- Perform further simulations for different scenarios with varied feedstock properties and hopper designs to guide successful design and operation of hopper
- Compare capabilities of two DEM modeling approaches (many representative spheres vs. fewer rod-like particles)

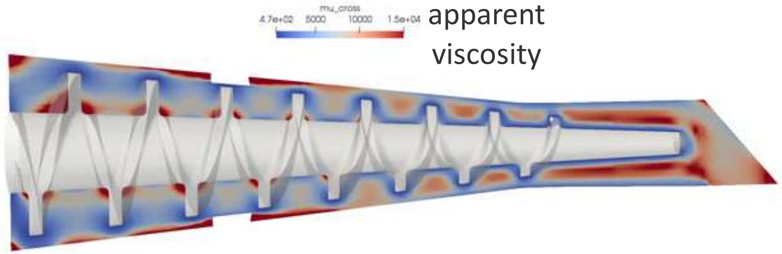
Task 2, Plug-Screw Feeder Operation (*progress/outcomes*)

Outcomes:

- Fitted biomass **compression** and **rheology** data to constitutive models
- OpenFOAM **CFD solver implemented** with equation-of-state for compressibility and density-dependent Cross model for non-Newtonian rheology.
- Simulated **torque** agreed with the experimental data (<20% error) for 2 screw feeders.



Parameter	Experiment	Simulation
Torque (N.m)	55,000±1000	60,000
Screw Speed (rpm)	38±1	38
Flow Rate (m^3/s)	0.033±0.001	0.03



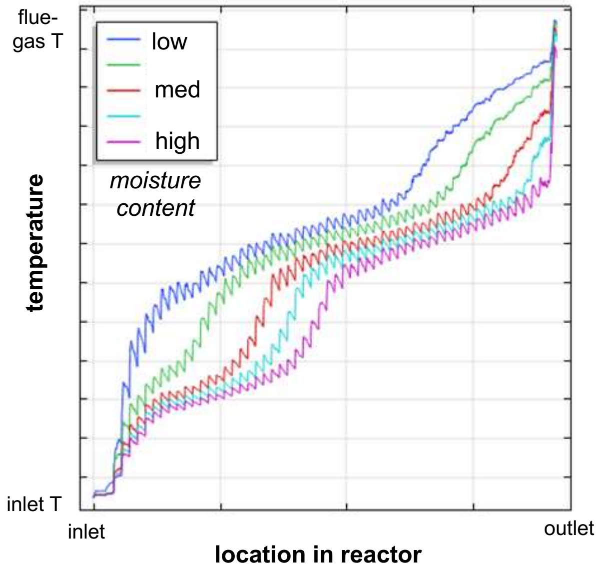
Remaining work:

- Perform **scenario simulations** to probe conditions that cause upsets
- Identify feedstock and operating conditions for **reliable performance**

Task 3, High temperature reactor modeling (*progress/outcomes*)

1. Impact of wood moisture content on temperature from inlet to outlet

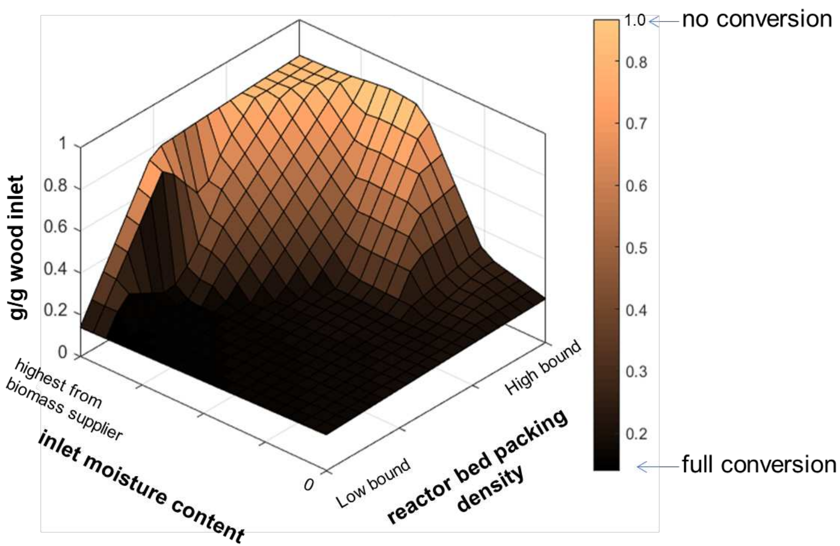
- Simulation results showing effect of feedstock moisture content on heat transfer through the bed was impactful to RRB
- Results showed the moisture significantly impacts required heat-up time and heat load



2. Impact of wood moisture content + bed packing on pyrolysis conversion

- Results showed reducing throughput with lower packing density can compensate for high moisture

Remaining work: Develop correlations from high-fidelity simulations



* some operational values not shown for client confidentiality reasons

Summary

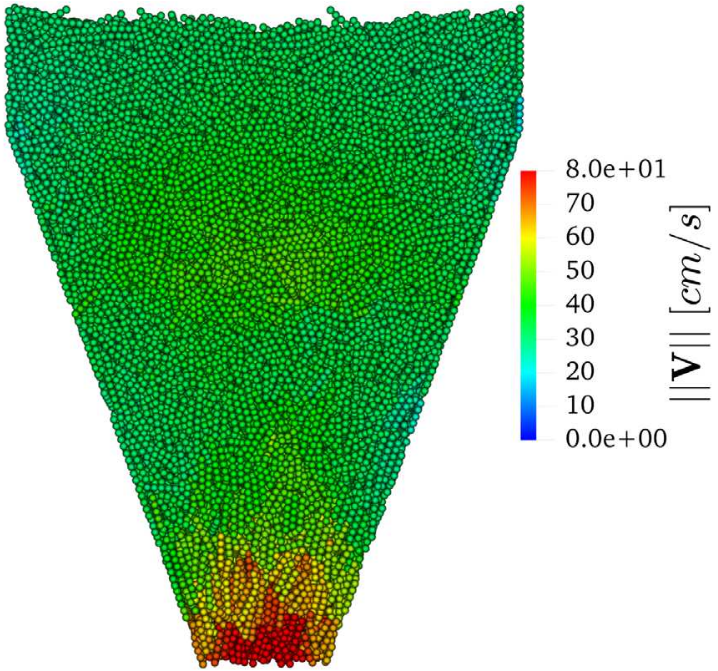
Overview: Physics-based computational modeling to address front-end feeding and reaction of an industrial biorefinery; these unit operations have experienced high failure rates in previous biorefinery startups

Management: High-impact team capable of executing the various parts of the project and managing risks

Approach: State-of-the-art computational modeling and simulations supported by rigorous material measurements and validation experiments

Impact: Optimize and de-risk operation of feeding and initial reaction of industrial biomass gasification process

Progress: Models developed and validated; Simulations are currently being used to identify reliable operating windows and sensitivities for RRB's process



Market Trends

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NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Value Proposition

- Optimize and de-risk deployment of an industrial biomass gasification process enabled by high-fidelity physics-based simulation

Key Accomplishments

- Models for all three areas have been validated
- Pyrolyzer simulations are informing RRB about how best to operate
- Silo and screw-feeder simulations targeting operational windows being performed now

Thank You

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We acknowledge funding from the **Advanced Demonstration and Optimization** platform of **BETO** and in-kind funding from Red Rock Biofuels, Jenike & Johanson, Valmet, and U Toledo.

A portion of the research was performed using computational resources sponsored by the Department of Energy's Office of Energy Efficiency and Renewable Energy and located at the National Renewable Energy Laboratory.

Transforming **ENERGY** through computational excellence

This project uses high performance computing resources located at Oak Ridge National Laboratory and provided by the Bioenergy Technologies Office.

NREL
Transforming ENERGY

Additional Slides

Quad Chart Overview

Timeline

- Start: January 1, 2018
- End: June 30, 2021

	FY20	Active Project
DOE Funding	$437,223	1,800,000
Project Cost Share	$109,306	$451,667

Project Partners

- NREL (44%)
- Red Rock Biofuels (12%)
- Jenike & Johanson (20%)
- Valmet (10%)
- U. Toledo (14%)

Project Goal

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

End of Project Milestone

(**Task 1**) Hopper design and operation. A suite of hopper simulations will be used to recommend optimal designs and operation. (**Task 2**) Screw feeder design and operation. A suite of commercial-scale plug-screw feeder simulations will be used to recommend optimal designs and operation. (**Task 3**) Deliver a correlation that may be used to estimate expected yields and optimal conveyor speeds for arbitrary feedstocks.

Funding Mechanism

Integrated Biorefinery Optimization (DE-FOA-0001689, 2017). Topic Area 4: Analytical modeling of solid materials (dry and wet feedstocks, and/or residual solids remaining in the process) and feeding systems to reactors

Responses to Previous Reviewers' Comments

Reviewer Comments	RESPONSE TO COMMENTS
A fundamental question in this project is that it is trying to both address an industrial optimization problem while addressing the novel use of complex computational techniques across three different unit operations. As a scientific endeavor is quite challenging, and while the potential exists to optimize the reactor feed line and performance, the project is overambitious. Validation of the model with experimental data is not clear, and real assessment of economic value is missing at this point. There are nuggets of interest - e.g. the screw feeder - but the overall project is disjointed and lacking the ability to make a strong case for itself. In addition, the quality of gasification modeling is somewhat limited. Lastly, we would like to see a direct involvement of equipment manufacturers.	We agree that our project is challenging and ambitious, but we feel that the role of National Lab projects is to address challenges of this magnitude. Although we will do our best to achieve the goals we proposed, there is always risk associated with scientific research. We expect to provide significant new methods and insights for feedstock feeding, even if we are not completely successful at using our models to optimize RRB's process. Experimental validation of the computational models is a key part of our work plan, and we apologize if that was not clear in the presentation. The equipment manufacturers Jenike and Johanson and Valmet are team members on this project. In addition, Red Rock Biofuels (RRB) have facilitated discussions between the team and TCG, the gasification-reactor vendor for RRB. Economic assessments performed by RRB have identified that reducing downtime associated with failures in the feeding system is critical to achieving economic targets; thus success in this project will provide substantial economic benefit.

Publications

- Xia, Y., Stickel, J. J., Jin, W., & Klinger, J. (2020). A Review of Computational Models for the Flow of Milled Biomass Part I: Discrete-Particle Models. *ACS Sustainable Chemistry & Engineering*, **8**(16), 6142–6156. https://doi.org/10.1021/acssuschemeng.0c00402
- Lattanzi, A. M., & Stickel, J. J. (2020). Hopper flows of mixtures of spherical and rod-like particles via the multisphere method. *AIChE Journal*, **66**(4), e16882. https://doi.org/10.1002/aic.16882
- Pecha, M. B., Arbelaez, J. I. M., Garcia-Perez, M., Chejne, F., & Ciesielski, P. N. (2019). Progress in understanding the four dominant intra-particle phenomena of lignocellulose pyrolysis: Chemical reactions, heat transfer, mass transfer, and phase change. *Green Chemistry*, **21**(11), 2868–2898. https://doi.org/10.1039/C9GC00585D

Presentations

- Ahsan, S. N., Sitaraman, H., Stickel, J., 2020, “Numerical Modeling of Woody Biomass Flow in Commercial-Scale Feeding System”, Presented at the 18th *Virtual International Congress on Rheology*, Rio De Janeiro, Brazil, December 2020.
- E. Akbari Fakhrabadi, C.A. Bullard, M. Rahimi, H. Sitaraman, J.J. Stickel, M.W. Liberatore. "Flow characterization of Lignocellulosic Biomass: An Experimental and Modeling Approach." Presented at the 18th *Virtual International Congress on Rheology*, Rio De Janeiro, Brazil, December 2020.
- E. Akbari Fakhrabadi, M.W. Liberatore, J.J. Stickel. "Flow Characterization of Fibrous Woody Biomass Using Experiments and Modeling." Presented at the *AIChE Annual Virtual Meeting*, San Francisco, CA, November 2020.
- E. Akbari Fakhrabadi, M.W. Liberatore. "Flow Behavior in Complex Fluids and Particulate Systems." Poster Presentation at the *AIChE Annual Virtual Meeting*, San Francisco, CA, November 2020.
- Hartford, Carrie E., "DEM Modeling Application to Biomass - Overcoming Handling Problems" presented virtually at the *International Conference for Sustainability Science & Engineering* (ICOSSE’20) AIChE, August 3, 2020
- Brennan Pecha, “How Biomass Burns and Char is Produced, Particle Size Optimum, Resulting Biochar Outcomes”, Presented Virtually at *Biomass to Biochar: Maximizing the Carbon Value*, April 2020
- Carrie Hartford and Jonathan Stickel. Strategic Partnership to Address Material Handling and Reactor-Feeding Challenges in the Biomass Industry. Presented at the *13th Annual International Biomass Conference and Expo*, Nashville, TN, February 2020
- Ehsan Akbari Fakhrabadi, Matthew W. Liberatore, Jonathan Stickel. Flow Behavior of Woody Biomass in a Lab-scale Compression Twin-screw Compounder. Poster presentation at the *Society of Rheology Annual Meeting*, Raleigh, NC, October 2019

Presentations, cont’d

- Mohammad Rahimi, Hariswaran Sitaraman, James Lischeske, David Sievers, and Jonathan Stickel. Computational Fluid Dynamics Simulation of Compressible Non-Newtonian Biomass in a Compression-Screw Feeder. Presented at the *AIChE Annual Meeting*, Orlando, FL, November 10, 2019
- Ehsan Akbari Fakhrabadi, Matthew W. Liberatore, Jonathan Stickel. Flow Characterization of Compressed Woody Biomass. Presented at the *AIChE Annual Meeting*, Orlando, FL, November 2019
- 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

Awards

- A poster presentation—Ehsan Akbari Fakhrabadi, Matthew W. Liberatore, Jonathan Stickel. Flow Behavior of Woody Biomass in a Lab-scale Compression Twin-screw Compounder—received 2 awards:
  - **First Place**: Career Development Event at EATON Corporations, November 2019.
  - **Second Place**: Detroit Science Symposium, December 2019.