NREL
Transforming ENERGY

Modeling Flow Behavior in a Disc-Refiner for the Deacetylation & Mechanical Refining (DMR) Process WBS#: 3.1.1.012

3/23/2020

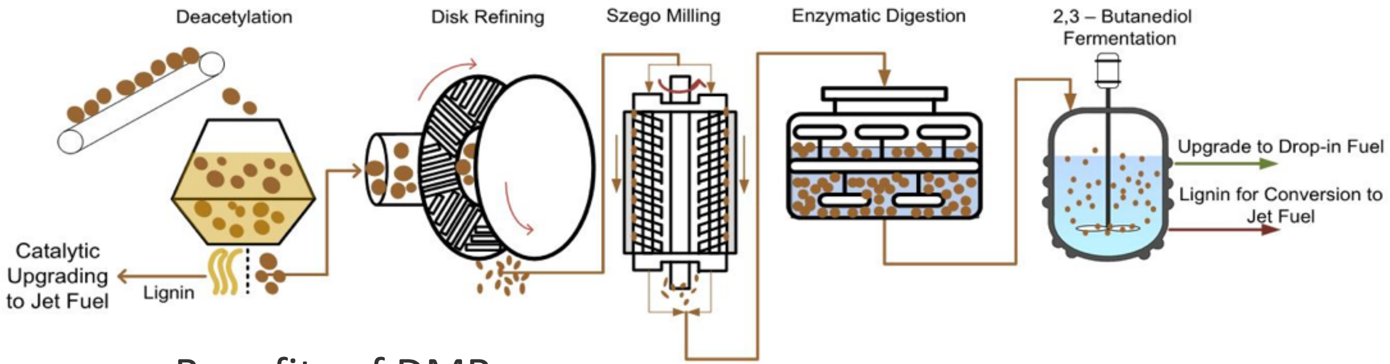
Conversion/Biochemical Platform

Xiaowen Chen & David Sievers

Catalytic Carbon Transformation and Scale-up Center

Project Overview

- Project Goals: Develop 3D advanced models that accurately predict refining power during disc-refining that will guide future disc plate designs and process parameter selections **to reduce energy consumption for GHG emission reduction** in the deacetylation and mechanical refining (DMR) process.



Benefits of DMR

- Low temp and atmospheric pressure
- Low-toxicity chemicals
- High sugar yield/titer at low enzyme loadings
- Uses industrial equipment
- Highly fermentable sugar and reactive lignin

Motivation of this project

- Fundamental science in disc refining poorly understood
- High refining energy reduces environmental benefits

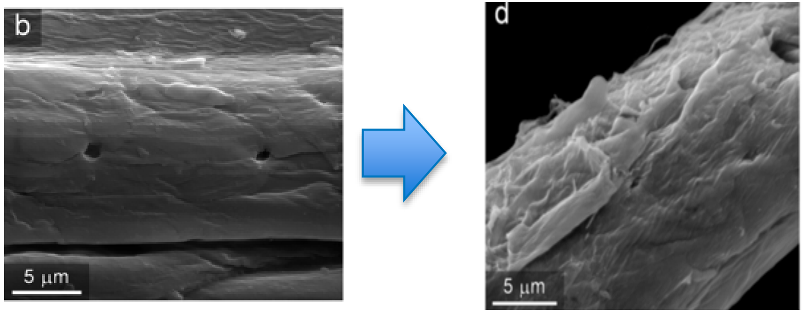
Project Overview

Increases surface area

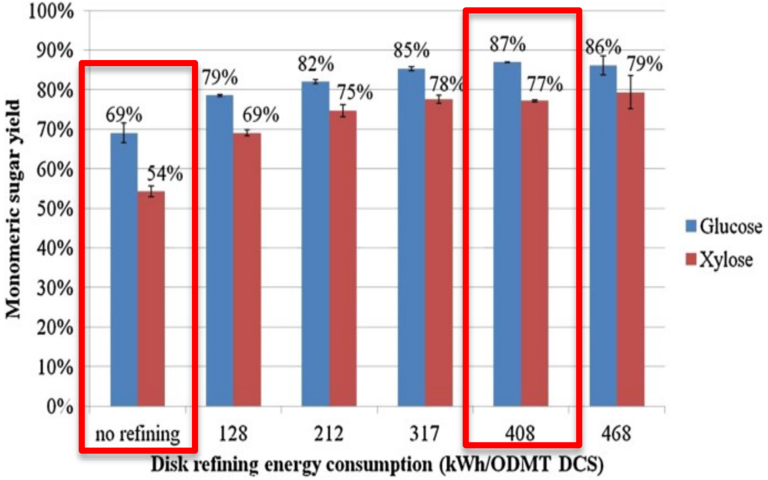
Introduces kinks and new reducing ends

Deacetylated CS

Disc refined DCS



Improves sugar yields



Project Goals

- Reduce the energy consumption to reduce GHG emissions
- Understand on how flow dynamics in disc refiner cause damages to the fiber
- Design plates targeting fiber damages instead of strengthening

Quad Chart Overview

Timeline
- Start date: 10/01/2019
- End date: 09/30/2022

	FY20	Active Project
DOE Funding	(10/01/2019 – 9/30/2020) *300K*	750K

Project Partners*
- Andritz

Barriers addressed
Ct-B. Efficient Preprocessing and Pretreatment

Project Goal
Develop models to establish scientific fundamentals for understanding and simulating the effects of refiner plate patterns and process parameters on the energy consumption and biomass digestibility in disc refining process for biofuel production.

End of Project Milestone
- The model will be used to predict the refining energy of one set of refiner plates for 22" disc refiner with less than 15% difference with experimental measurement.
- Demonstrate ≥ 5% reduction in MSSP by reducing refining energy using the plates and refining conditions guided by model predictions.

Funding Mechanism
SDI seed project.

Market Trends

Product	Gasoline/ethanol demand decreasing, diesel demand steady
Product	Increasing demand for aviation and marine fuel
Product	Demand for higher-performance products
Product	Increasing demand for renewable/recyclable materials
Feedstock	Sustained low oil prices
Feedstock	Decreasing cost of renewable electricity
Feedstock	Sustainable waste management
Feedstock	Expanding availability of green H_2
Feedstock	Closing the carbon cycle
Capital	Risk of greenfield investments
Capital	Challenges and costs of biorefinery start-up
Capital	Availability of depreciated and underutilized capital equipment
Social Responsibility	Carbon intensity reduction
Social Responsibility	Access to clean air and water
Social Responsibility	Environmental equity

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

Value Proposition

- This project directly supports BETO's multi-year plan to reduce energy consumption for environmentally friendly biofuel and bioproduct processing through advanced modelling and fundamental understanding of the disc-refining process.

Key Differentiators

- 3D-CFD models that have rarely been used in studying disc refining process
- Validating models using experimental data
- Capable to scale up the model for use in commercial size disc refiner
- Target: Weakening fibers through new plate designs (instead of strengthening fibers in traditional pulping industries)

1. Management

ANDRITZ

Disc refiner modelling

PI: Xiaowen Chen,

David A. Sievers

Task 1:

Disc refiner model development

Task 2:

Energy consumption and validation

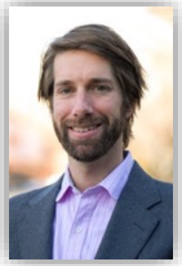
Collaboration:

Low Temperature Advance Deconstruction (WBS #: 2.2.3.100)

Pilot Scale Integration (WBS#: 2.4.1.301)

Feedstock Conversion Interface Consortium

Xiaowen Chen



David Sievers

Yudong Li

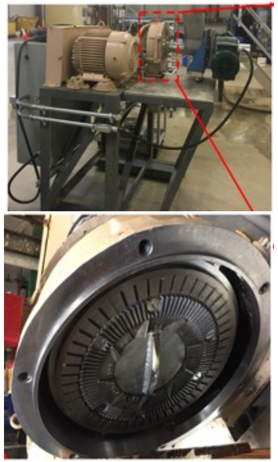
Expertise: chemical engineering, process design, automation, data mining, and modeling

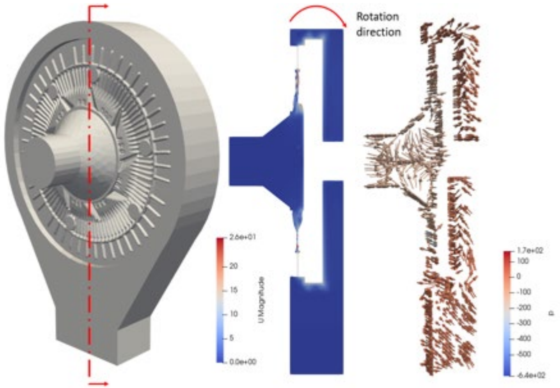
Risks

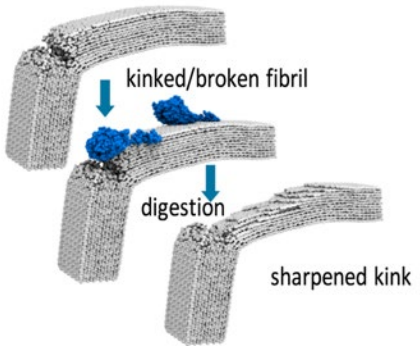
High computational power requirement due to high complexity

Reliable literature and fundamental science is not widely available

2. Approach







Ciesielski et al., PNAS 2019 116 (20)

- Physically enclosed and cannot be observed
- Many variables: plate designs, plate gaps, rotational speed, feed rate, feed solids%, initial biomass attributes, etc.

- Use 3D CFD model to simulate and understand flow behavior, shear energy, and power consumption
- Validate the model with experimentally measured energy consumption
- Use models to select best disc-refiner geometry designs *in silico* (targeted approach)
- Understand the fundamental relationships between fiber damage (enabling enz. hyd.), energy use, and shear stress.

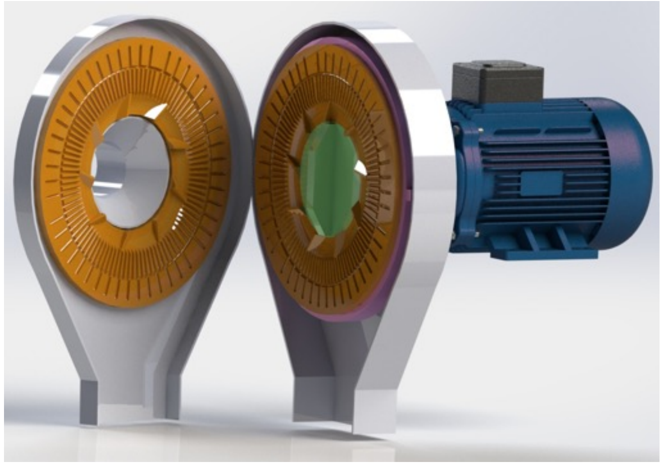
2. Approach (continued)

Modelling approach

- **Scan to CAD**: The geometric features of the refiner plate plays a critical role in biomass refining. We use a 3D scanner to obtain high-fidelity 3D renderings for model development.

Disc-refiner

3D scanner

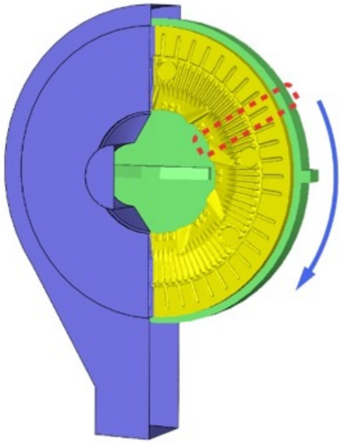


Disc-refiner model

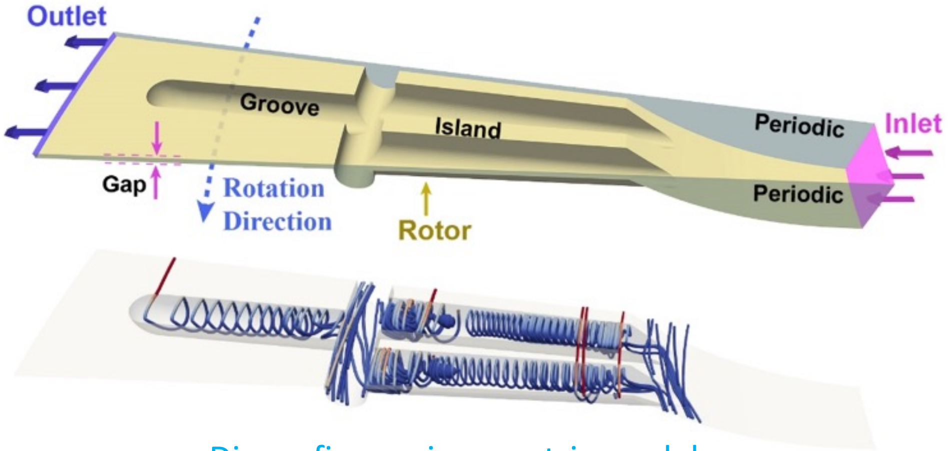
2. Approach (continued)

Modelling approach

- **Complexity reduction** (*Risk mitigation*): High geometric complexity of the full disc refiner. We took advantage of the axisymmetric characteristics to reduce model complexity and model the smallest repeating section.



Disc-refiner model



Disc-refiner axisymmetric model

Geometry:	full refiner geometry	vs.	< 1% of full refiner geometry
Computational cells:	> 200M	vs.	~ 2M
Resources:	NA	vs.	~ 64x20 core hours (3.0 GHz) per run

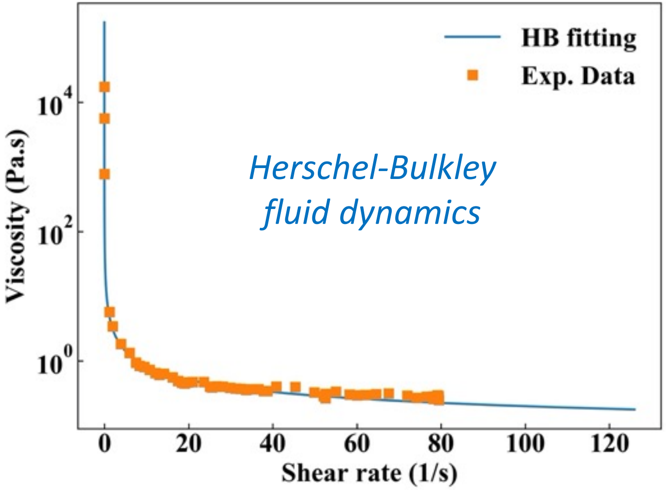
2. Approach (continued)

Experimental approach

- **Physical properties:** Biomass slurry response to mechanical deformation is critical in modelling energy consumption. A rheometer is employed to provide detailed characterization of the biomass slurry rheological behavior.

- **Model Validation**: Energy consumption of the disc-refiner machine is recorded real-time to validate the model-predicted energy consumption.

Rheometer



Biomass slurry rheological behavior

3. Impact

- Reduce GHG Emissions—lower electrical demand of biofuel/chemical process, repurpose existing pulp & paper machines for deconstruction—also reduces overall costs

- Help reduce GHG Emissions of pulp & paper—models and fundamental knowledge can direct efficiency improvements here also

- New fundamental understanding leads to publications & patents—also unlocks future use beyond herbaceous biomass, such as MSW

Publication: *Modelling the disc refining of herbaceous lignocellulosic biomass in deacetylation and mechanical refining pretreatment: energy consumption prediction and validation* (in preparation)

Partnership:

- *Providing new 22" refiner for NREL*
- *Manufacturing custom plates*
- *Bring new designs to market*

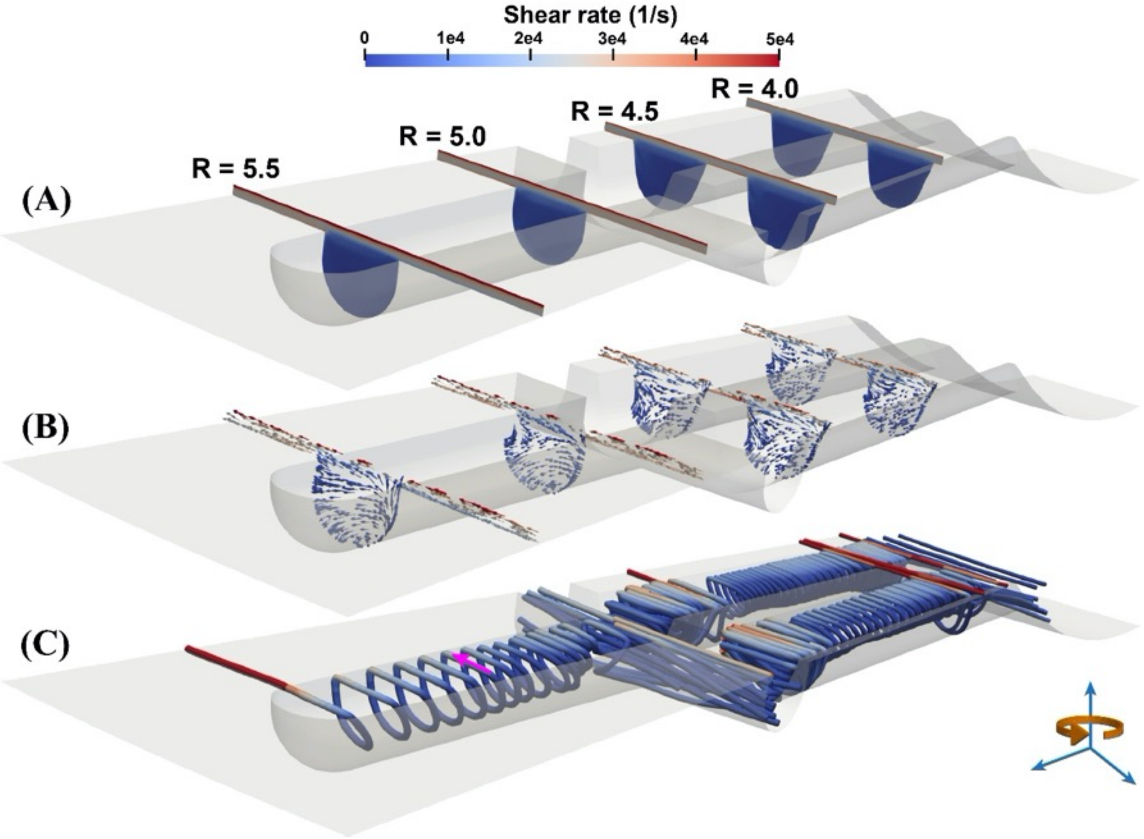
4. Progress and Outcomes

Major achievements include

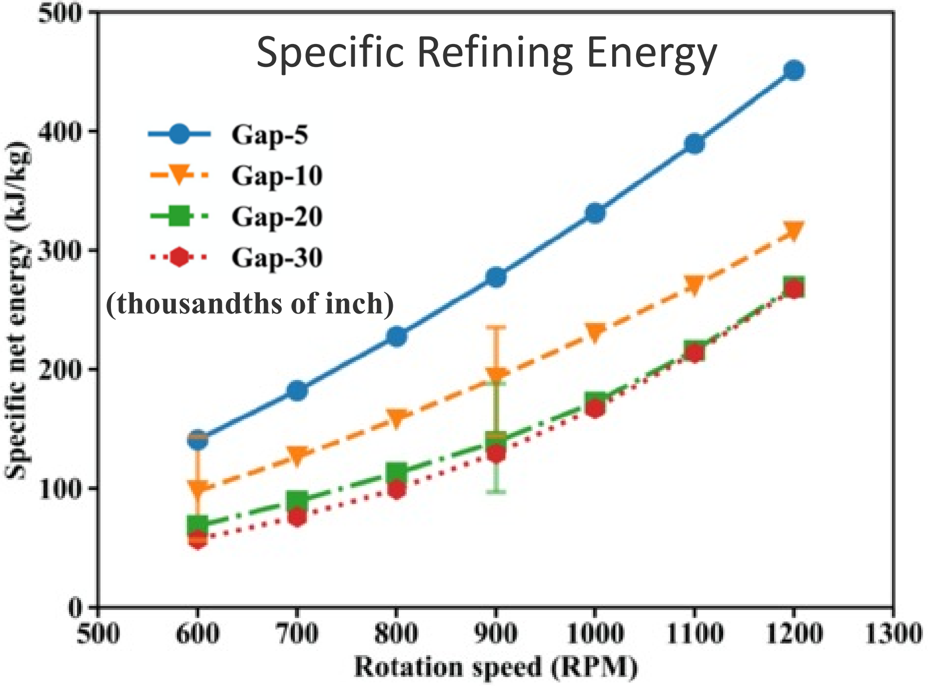
- This project **achieved all planned milestones, on schedule**.
- **Literature review** and 3D refiner geometric model construction.
- **Risk mitigation** has been employed to address computational complexity of the full refiner model by taking advantage of repeating symmetry.
- **Simulations were successfully performed** based on experimental conditions.
- **Model validated** by experimental measurements. Accurate prediction of disc-refining power **within 5%** of experimental results.

4. Biomass slurry flow behavior — model insights

- Shear occurs at refiner plate gap—higher severity at farther radial positions.
- Recirculation occurs in the grooves, which increases residence time of material between the plates. Recirculation aids the formation of fiber flocs that result in fiber disruption.



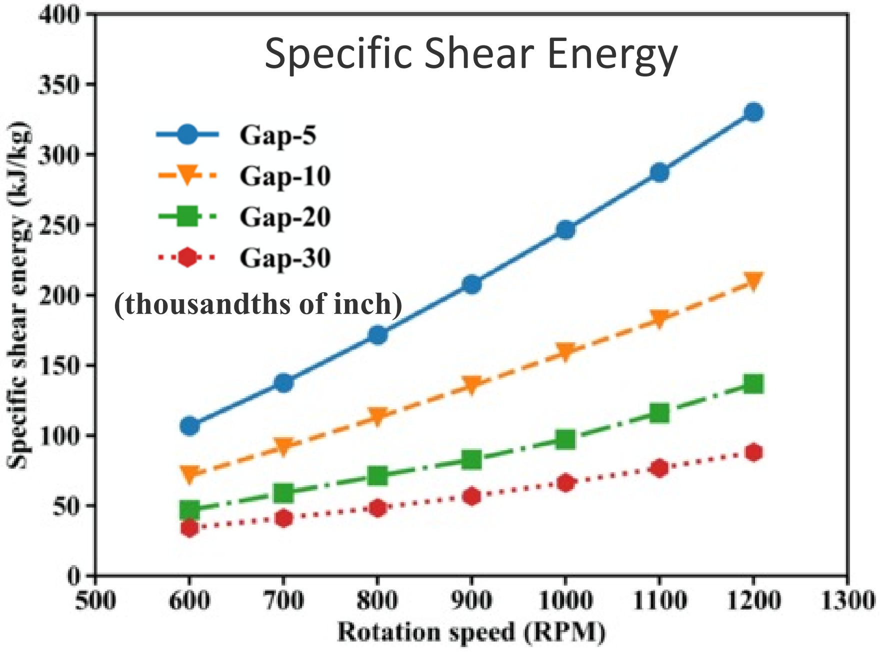
4. Model validation and results



Simulation results validated with experimental data (points with error bars)

- Simulation (lines with symbols) accurately (< 5% error) predicted the refining power consumption compared with experimental results.
- Faster rotation speed and narrower gap requires higher energy.

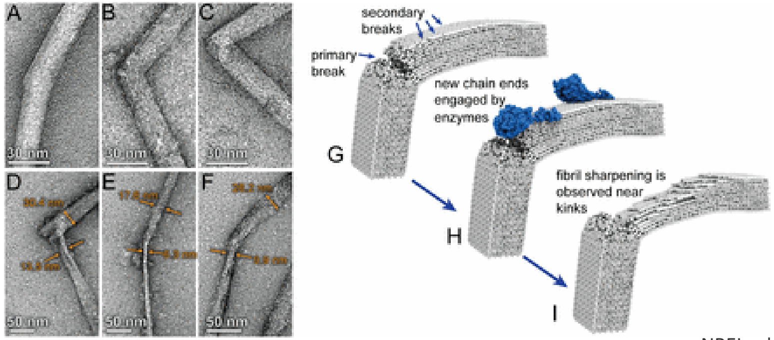
4. Model results — Shear



Mechanical deformation associated with kinking & fiber breakage—ultimately better digestibility

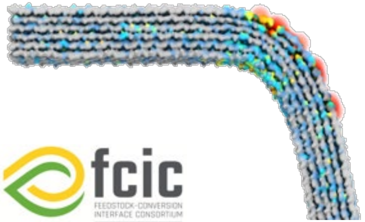
[Ciesielski PNAS 2019 116 (20) 9825-9830]

- *Shear energy* is the refining energy utilized shearing the biomass particles. <u>Predicted by simulation but not directly measurable.</u>
- Faster rotation speeds and narrower gaps impose higher shear to biomass slurry.
- *We now seek understanding how shear is related to kinking and defibrillation*



Future Plans

- *Publication (in works currently)*
- Elucidate the fundamental relationships between fiber damage, energy use, and shear stress by incorporating mesoscale models with CFD-DEM. Enables targeted selection of plate geometries.
- Simulate the larger, 22-inch disc-refiner (to be installed late 2021) using the model and compare with experimental results. Further scientific understanding of scale-up.



fcic
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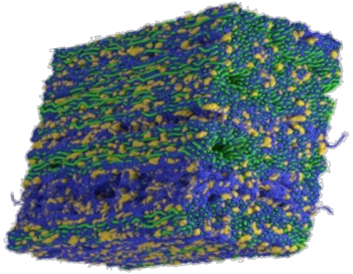
Molecular/Macromolecular models relate nanomechanics to reactive defect formation

Mesoscale models capture response of biopolymer matrix to chemical + mechanical deconstruction to inform bulk CFD



Ciesielski ongoing work in FCIC subtask 5.4

NREL's 22-inch Disc-Refiner

Summary

1. **Management**
   – Directly addressing BETO's request to reduce GHG of DMR process
   – Risk mitigation plan was successfully deployed to achieve project goals
2. **Approach**
   – Developing 3D CFD models to simulate and understand flow behavior, shear energy, and power
   – Model complexity reduction through symmetry, Validation through experiments
   – Use model to select best disc-refiner geometry designs *in silico* (targeted approach)
   – Elucidate fundamental refining mechanisms (fiber damage vs. energy use vs. shear stress)
3. **Impact**
   – Reduction of GHG, reduction of costs (lower energy, also repurposing of existing machines)
   – Help existing industry (pulp & paper) also reduce GHG
   – Publications & potential patents on new designs
   – Deploy new designs to market through our industry sector leader and partner: Andritz
4. **Progress and outcomes**
   – High-fidelity model developed based on NREL's 12-inch disc-refiner
   – The model accurately predicted energy consumption at different conditions with less than 5% difference from experimental measurements
   – Shear energy now can be simulated based on geometry and process parameters

Thank you

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NREL Transforming ENERGY

Market Trends

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	Demand for higher-performance products
	Increasing demand for renewable/recyclable materials
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	Environmental equity

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Value Proposition

- This project directly supports BETO's multi-year plan to reduce energy consumption for environmentally friendly biofuel and bioproduct processing through advanced modelling and fundamental understanding of the disc-refining process.

Major Achievement

- A 3D high-fidelity model was developed based on NREL's 12-inch disc-refiner.
- Simulations were performed at different disc refining parameters (gap size and rotation speed) with respective shear energy computed.
- The model accurately predicted energy consumption at different conditions with less than 5% difference compared with experimental measurements.