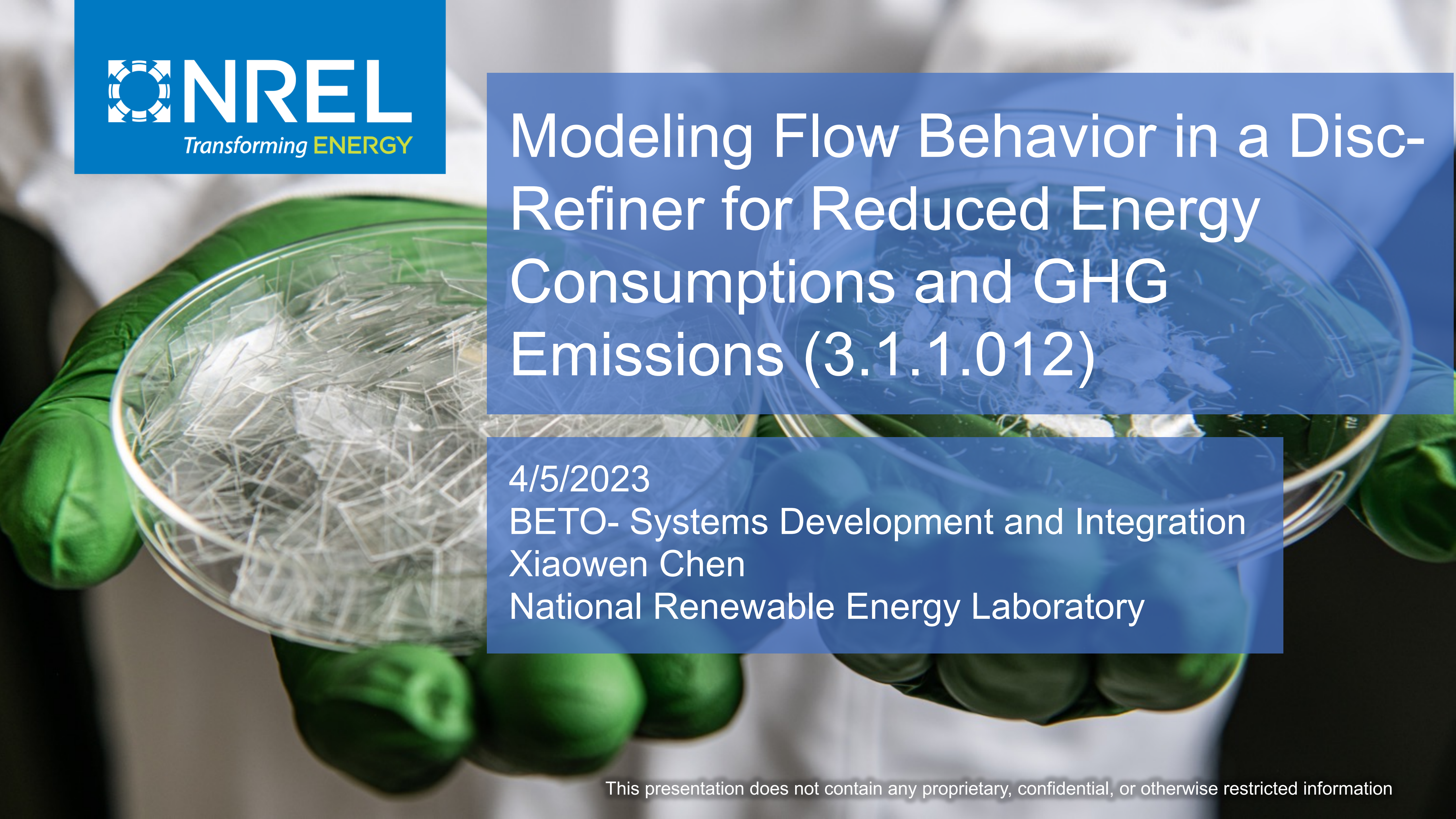
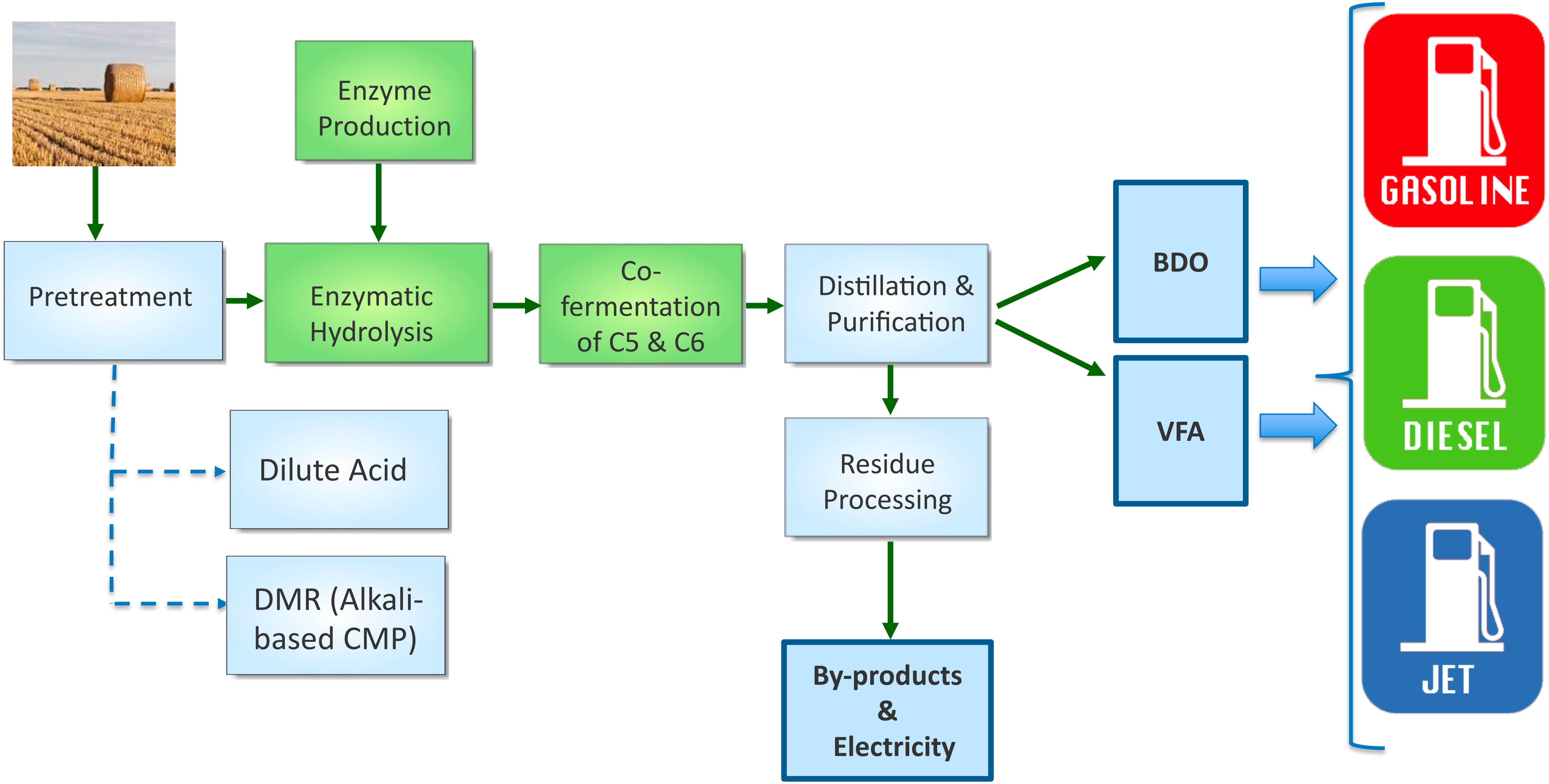


Modeling Flow Behavior in a Disc-Refiner for Reduced Energy Consumptions and GHG Emissions (3.1.1.012)

4/5/2023
BETO- Systems Development and Integration
Xiaowen Chen
National Renewable Energy Laboratory

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project Background



Enzyme Production

Pretreatment

Enzymatic Hydrolysis

Co-fermentation of C5 & C6

Distillation & Purification

Residue Processing

By-products & Electricity

Dilute Acid

DMR (Alkali-based CMP)

BDO

VFA

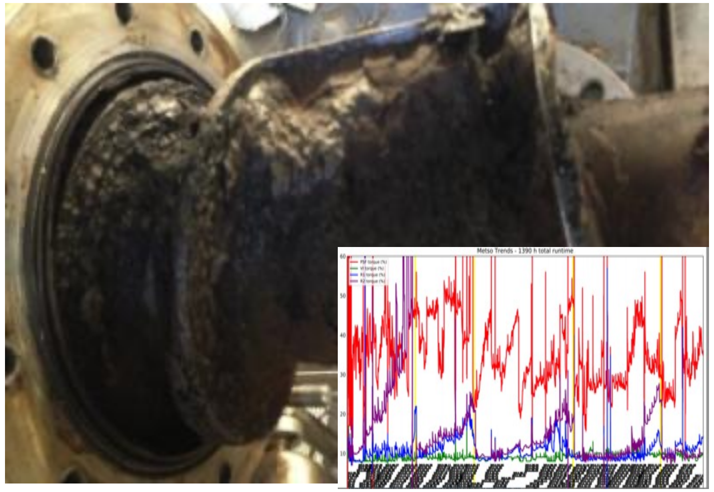
GASOLINE

DIESEL

JET

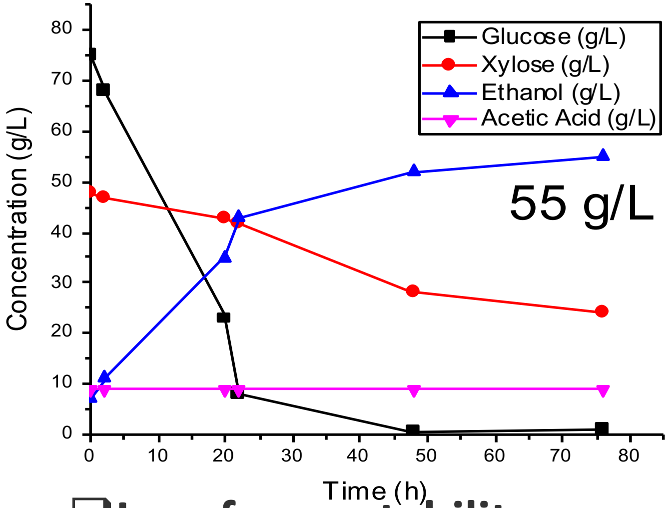
Why NOT Dilute Acid?

☐**Unable to feed or steam blow back**



☐**Accumulating chars**

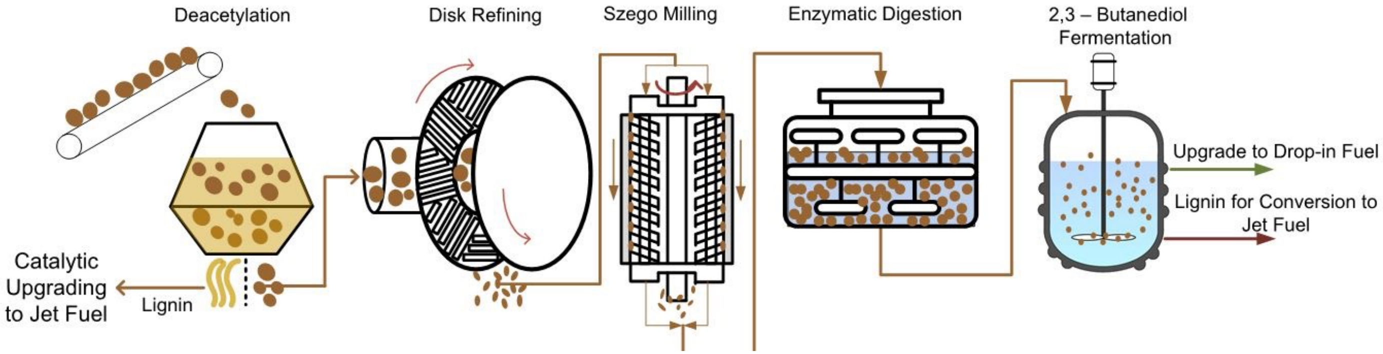
☐**Wearing out feeding screws**

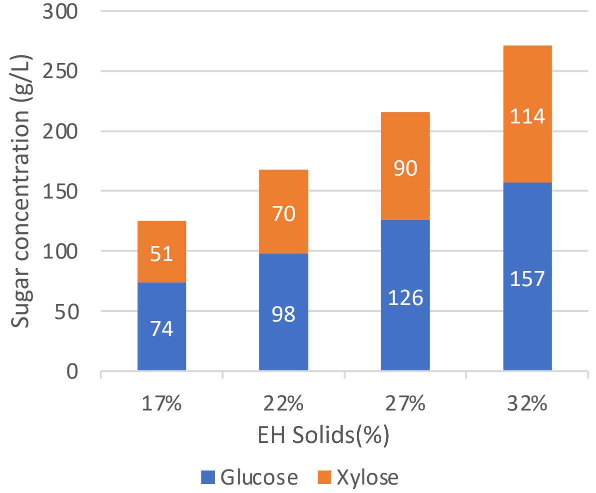


☐**Low fermentability**

Why DMR?

The Deacetylation and Mechanical Refining process

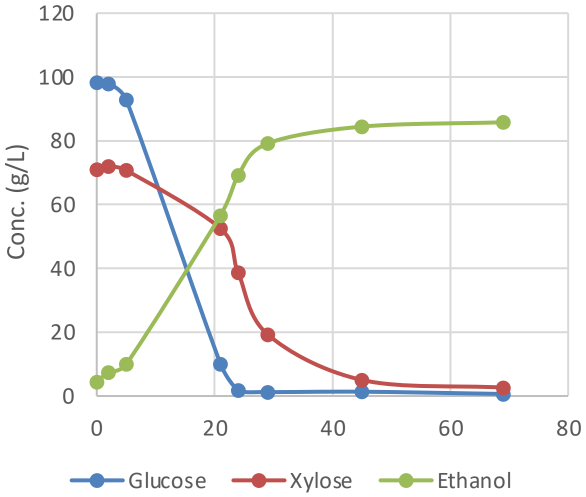




Advantages & Importance

- Low Temp
- Atmospheric Pressure
- No toxic chemicals
- Uses industrial equipment
- High sugar yield/titer
- Low enzyme loadings
- Highly fermentable
- Reactive Lignin
- Does not contain sulfur

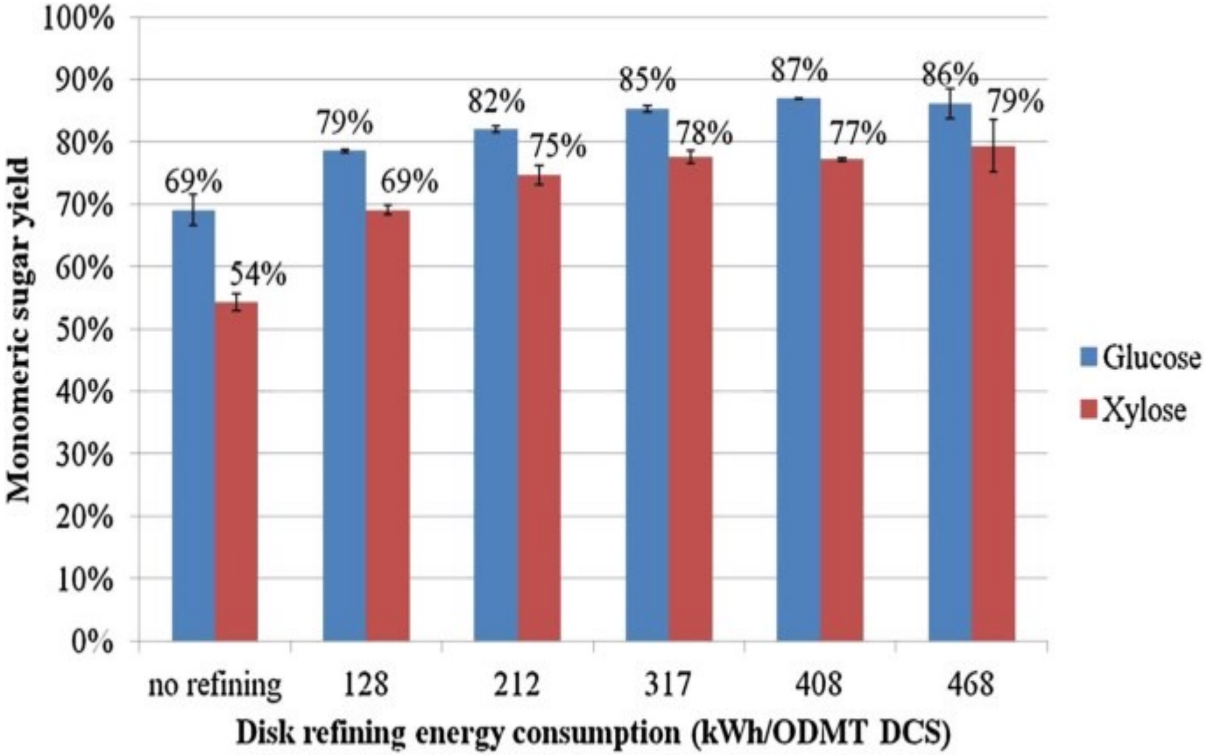
- ↘ Capital cost
- ↗ Operation reliability
- ↘Maintenance cost
- Scalable and Industry relevant
- ↗ Revenue
- ↘Operational cost
- ↗ Revenue and value-added products
- ↗ Catalyst life

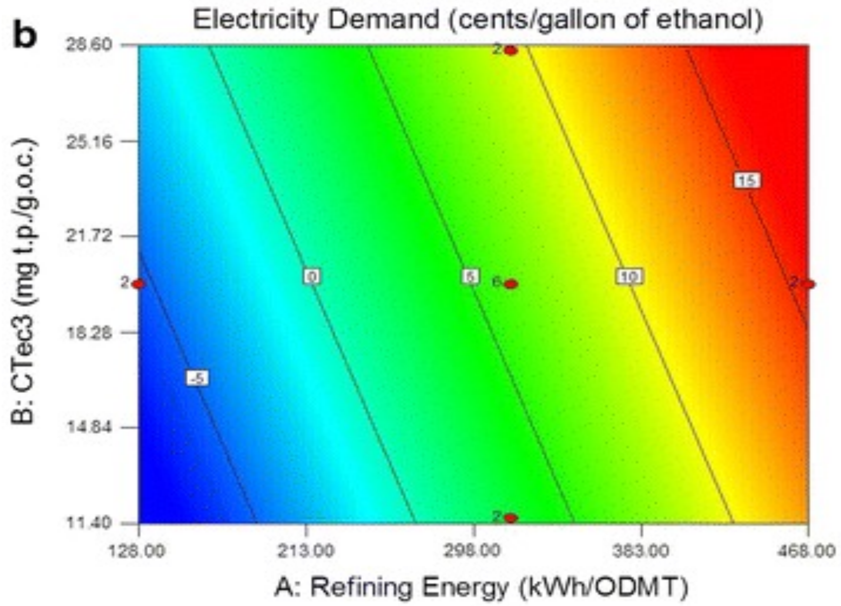


Project Overview

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

Disk refining improves sugar yields by as much as 20%, while consuming ~ 5 – 15 kWh/GGE (1 GGE contain ~40 kWh).

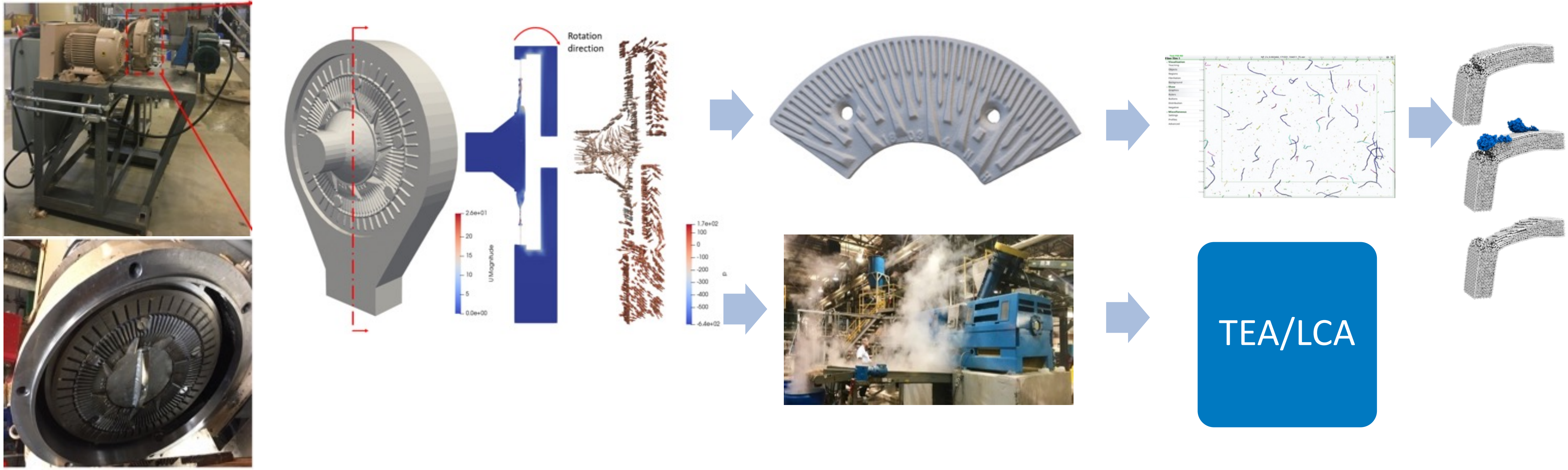




Reducing refining energy is critical to achieve 70% GHG emissions reduction of lignocellulosic biorefinery.

- This project aims to reduce >15% refining energy (SOT19) with the use of 22" disk refiner

Approach



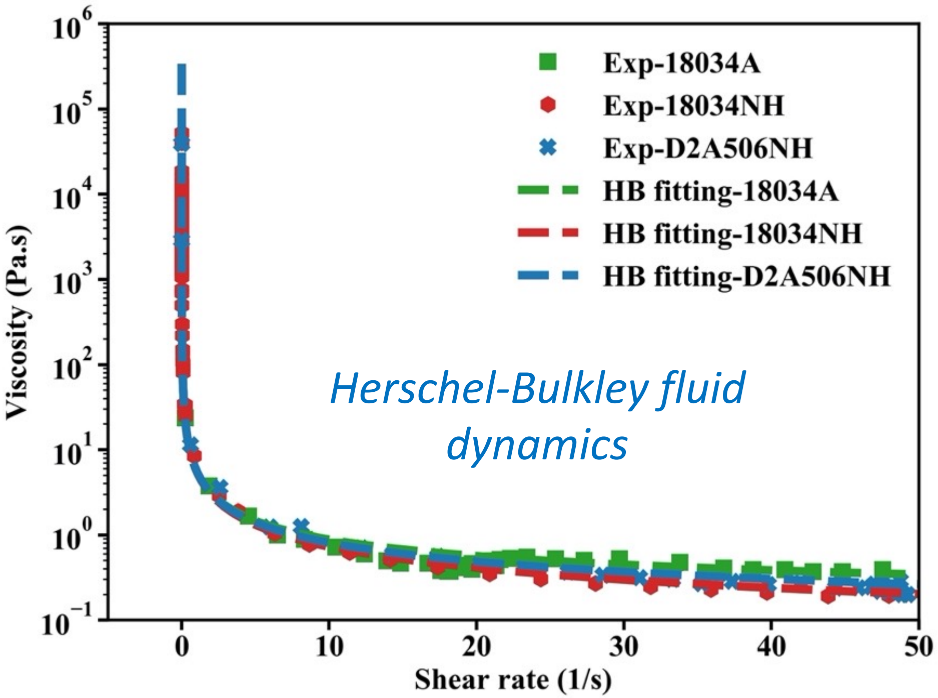
Advancing the current SOT on disk refining technology

- Develop an experimentally validated 3D CFD model to understand flow behavior, and predict power consumptions
- Reduce refining energy by optimizing refining conditions and refining plate geometries
- Predict refining energy and performance at larger scales using the 3D CFD model
- Enable the coupling of CFD model with mesoscale simulation framework to elucidate refining mechanism optimized for enzymatic hydrolysis
- Inform the TEA and LCA models and find the major economic and environmental impact drivers

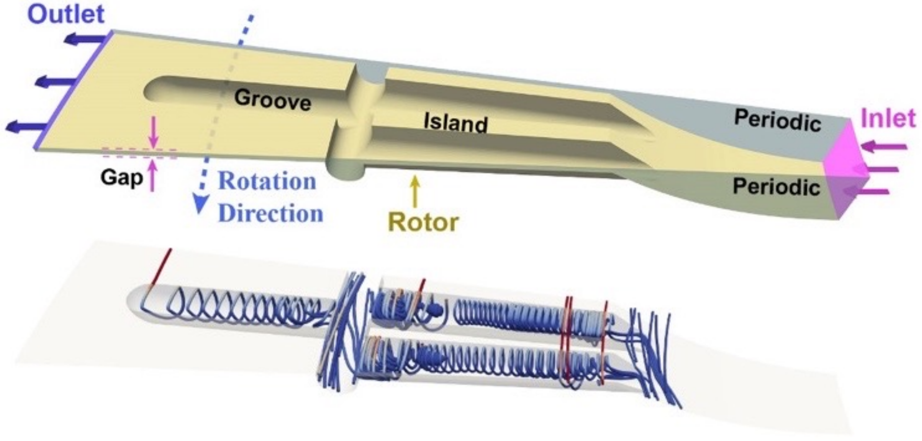
Potential Innovations

- Enable the design of energy efficient disk plates for biorefinery industry purpose

Approach (continued)



Herschel-Bulkley fluid dynamics



Risks and Mitigation Strategy

- Risk 1 : High solids disk refining (>20%) does not form a consistent flow inside the refiner
  - Mitigation: Reduced the solids loading of disk refiner to 3% for modeling purpose
- Risk 2: High computational power requirement for whole plate modeling
  - Mitigation: We modeled a section of the geometry taking advantage of its symmetric characteristics which greatly reduces computational time without sacrificing model fidelity.

Collaborations

- We are working with Andritz to seek opportunities for manufacturing biorefinery-specific plate based on the model and experiment results.

Progress and Outcomes (PO) 1 : Rotational Speed

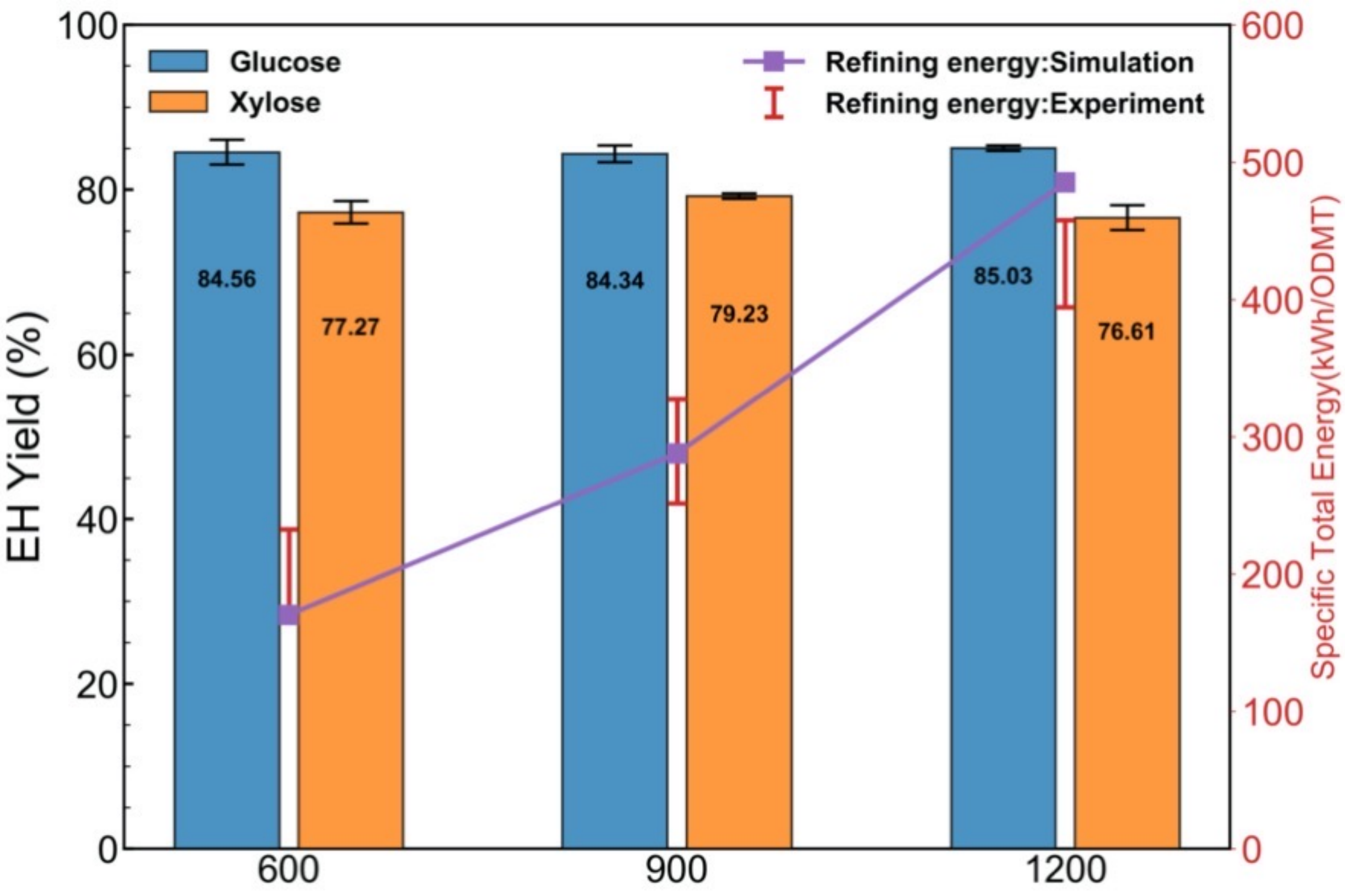


Plate: 18034A; Gap: 0.01 inch; Consistency: 3 wt%; Feed: 5.4kg/hr

- Refining energy increases with increasing rotation speed, which was used in cross validation of the 3D-CFD model.
- Sugar yields didn't benefit from the increasing rotation speed, for the feeding rate and consistency.
- Our hypothesis is that the fiber delamination reached a plateau even at lower rotation speed, given the constant plate gap and feeding rate/consistency.
- Higher energy used at higher rotational speed is likely to be wasted in heating up the slurry

PO2: Plate Gap

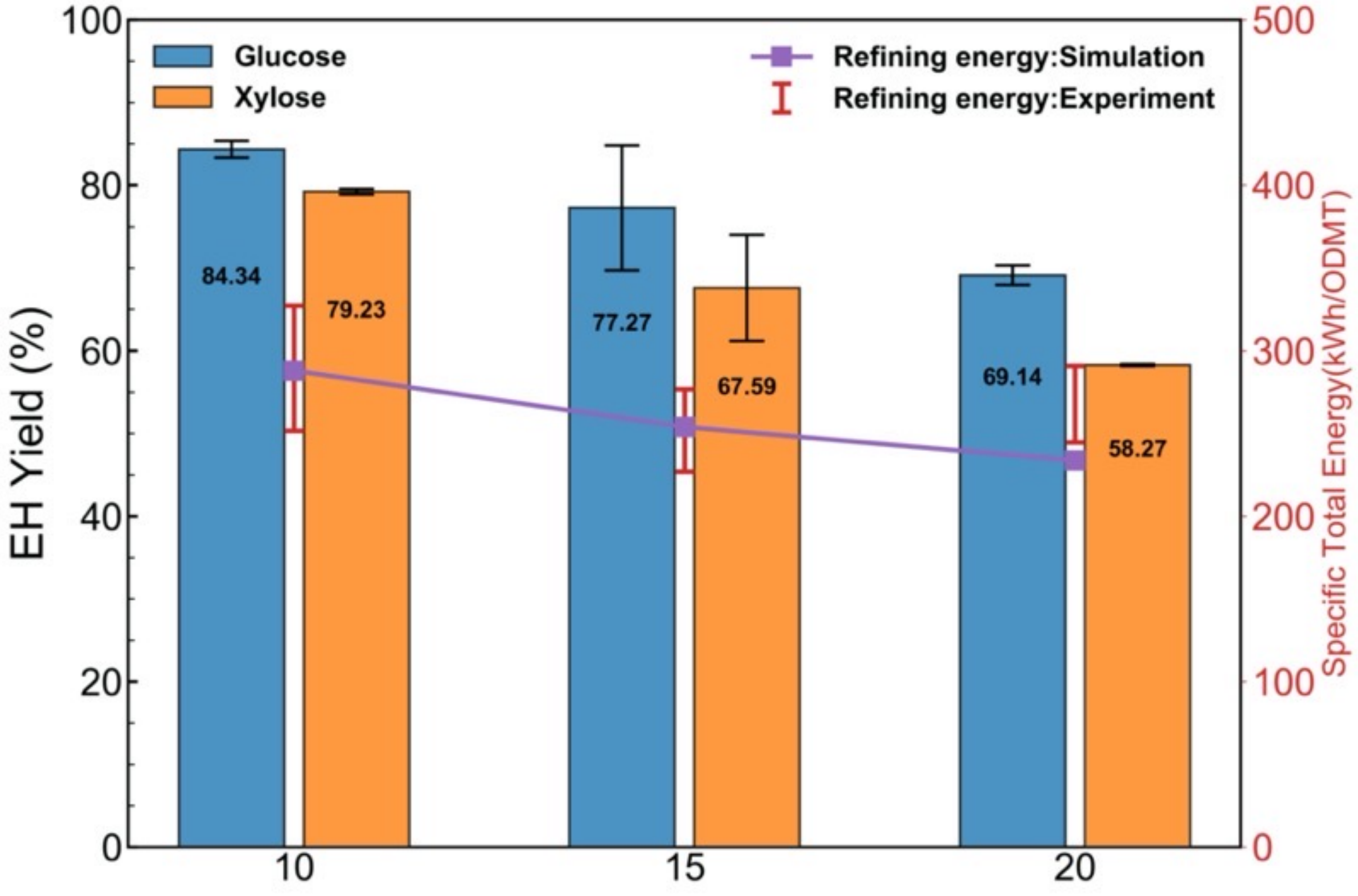
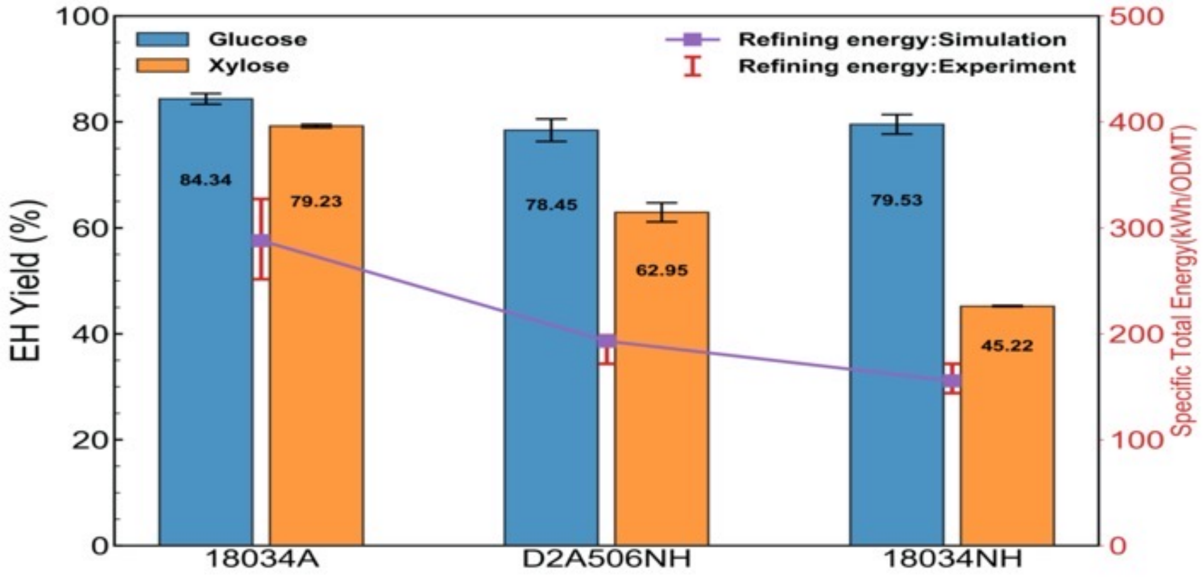
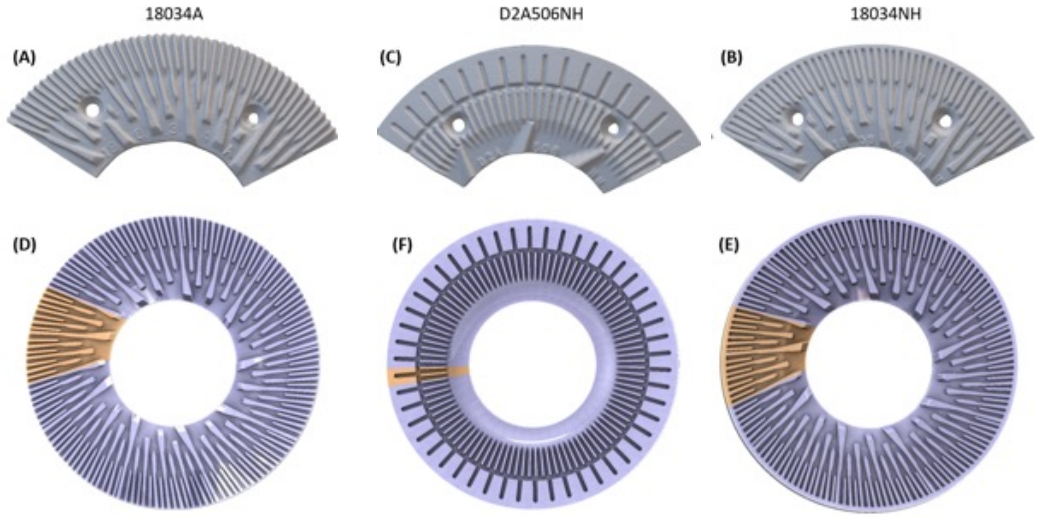


Plate: 18034A; Rotation: 900RPM; Consistency: 3 wt%; Feed: 5.4kg/hr

- Refining energy decrease with increasing gap
- Sugar yields decreases with increasing gap
- Plate gap affects more on sugar yield (up to 18% decrease on glucose) and less on refining energy (up to 8% decrease on refining energy)
- Lower plate gap results in more fiber bar interactions, leading to more internal delamination of second wall structure

PO3: Plate Geometry

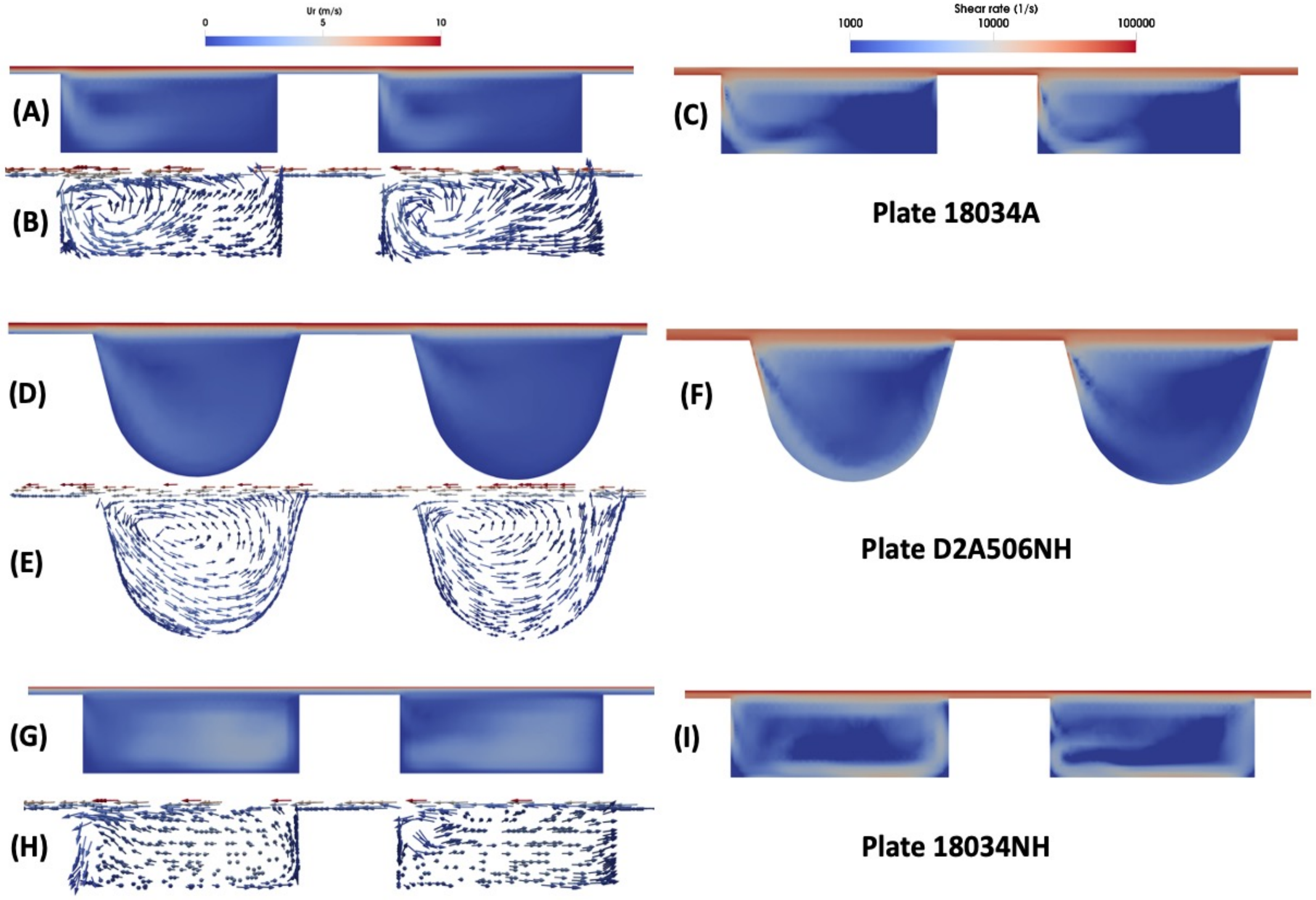




Gap: 0.01inch; Rotation: 900RPM; Consistency: 3 wt%; Feed: 5.4kg/hr

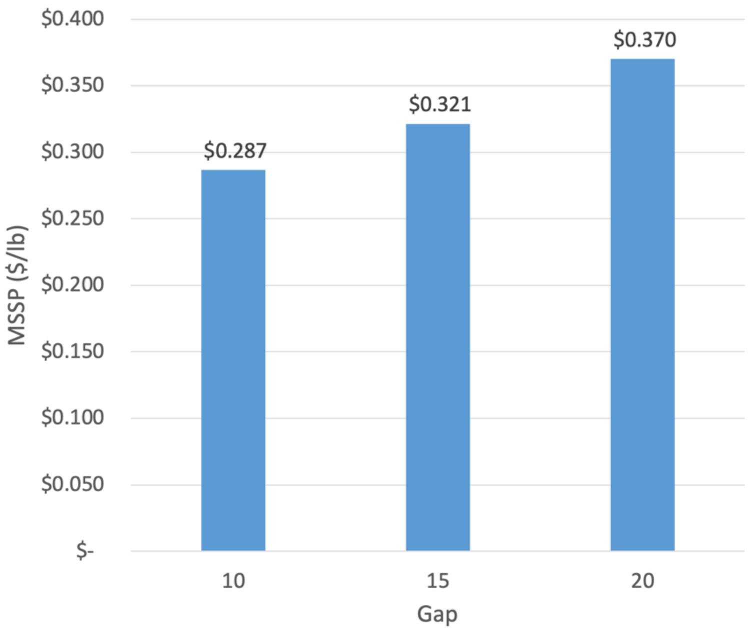
- Proper plate design is critical for milling the biomass uniformly and produce similar sugar digestibility of the biomass.
- Proper plate design could allow fiber to flow in a controlled fashion through the disk plates and avoid back flow. Efficient flow reduces energy need.
  - **Valmet create 6 GWh in electricity saving for disk refining in pulping industry**
- Plate geometry designs affect refining energy more than sugar yields. (84% less energy consumption comparing 18034NH with 18034A, a type of open groove designs used in pulping refiners)
- Optimizing plate designs will lead to reduced refining energy and related GHG emissions without dramatically decrease sugar yields.

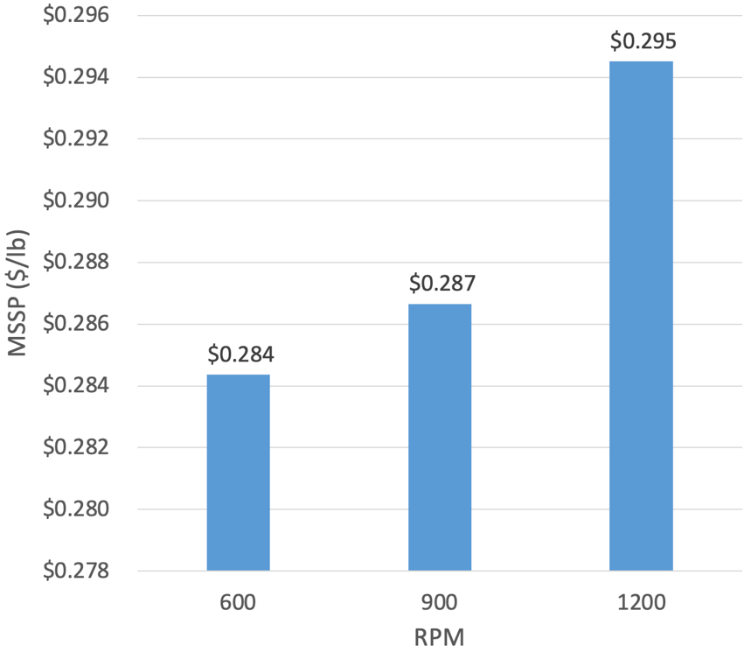
PO4: Flow Pattern and Sugar Yield

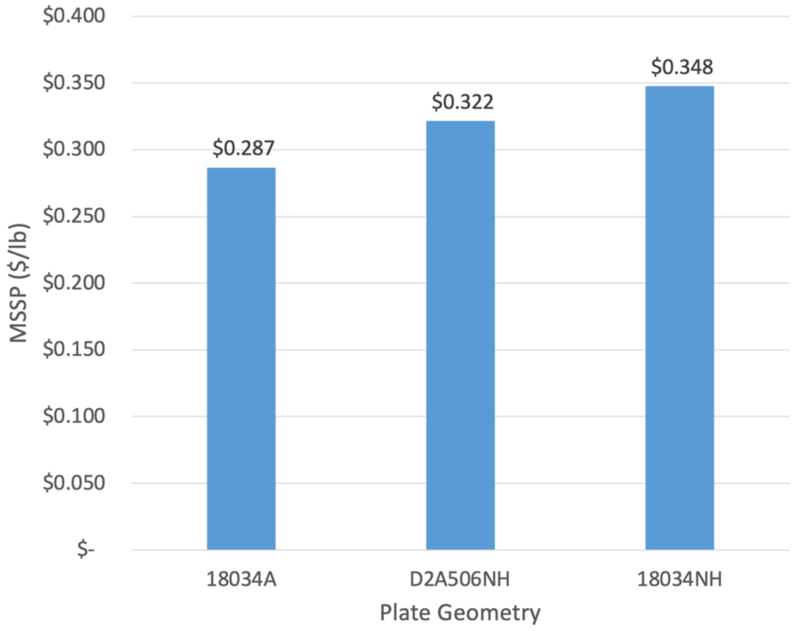


- Circulation intensity :18034A > D2A506NH > 18034NH
- Positive correlation between circulation flow intensity and shear rate with the enzymatic sugar yields

PO5:Minimum Sugar Selling Price



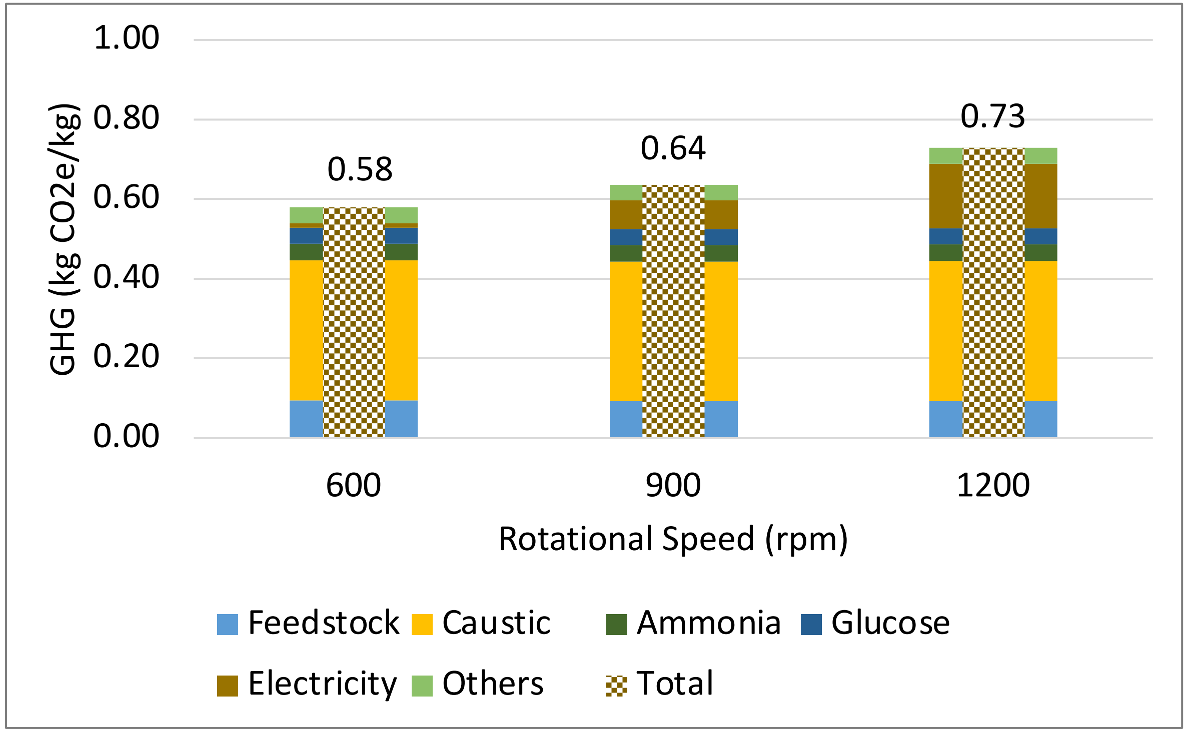


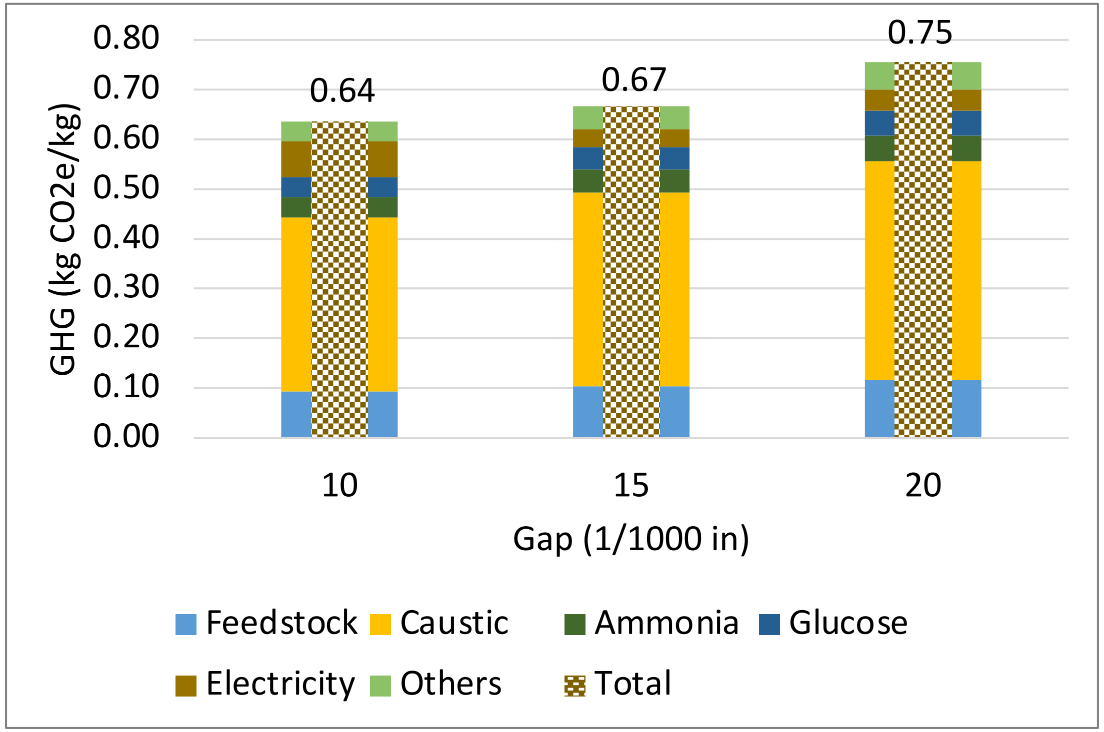


	Energy Consumption	Sugar Yield	MSSP
Gap↘	↗	↗	↘
RPM↘	↘	↔	↘

- MSSP: 18034A <D2A506NH<18034NH.
- MSSP: Sugar yield > Energy consumption

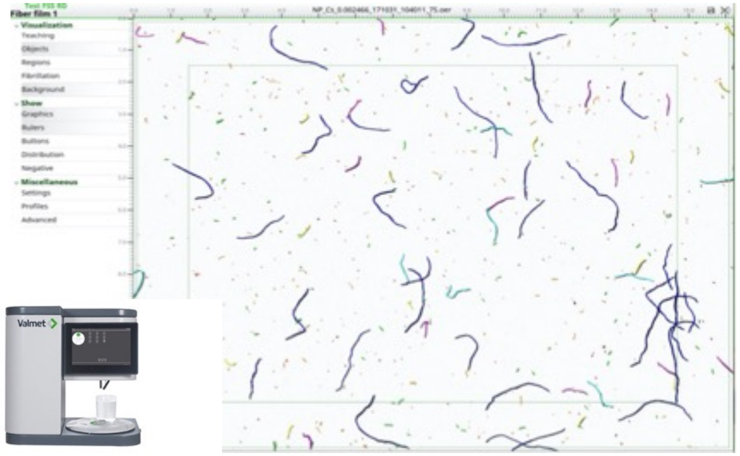
PO6: Life Cycle Analysis

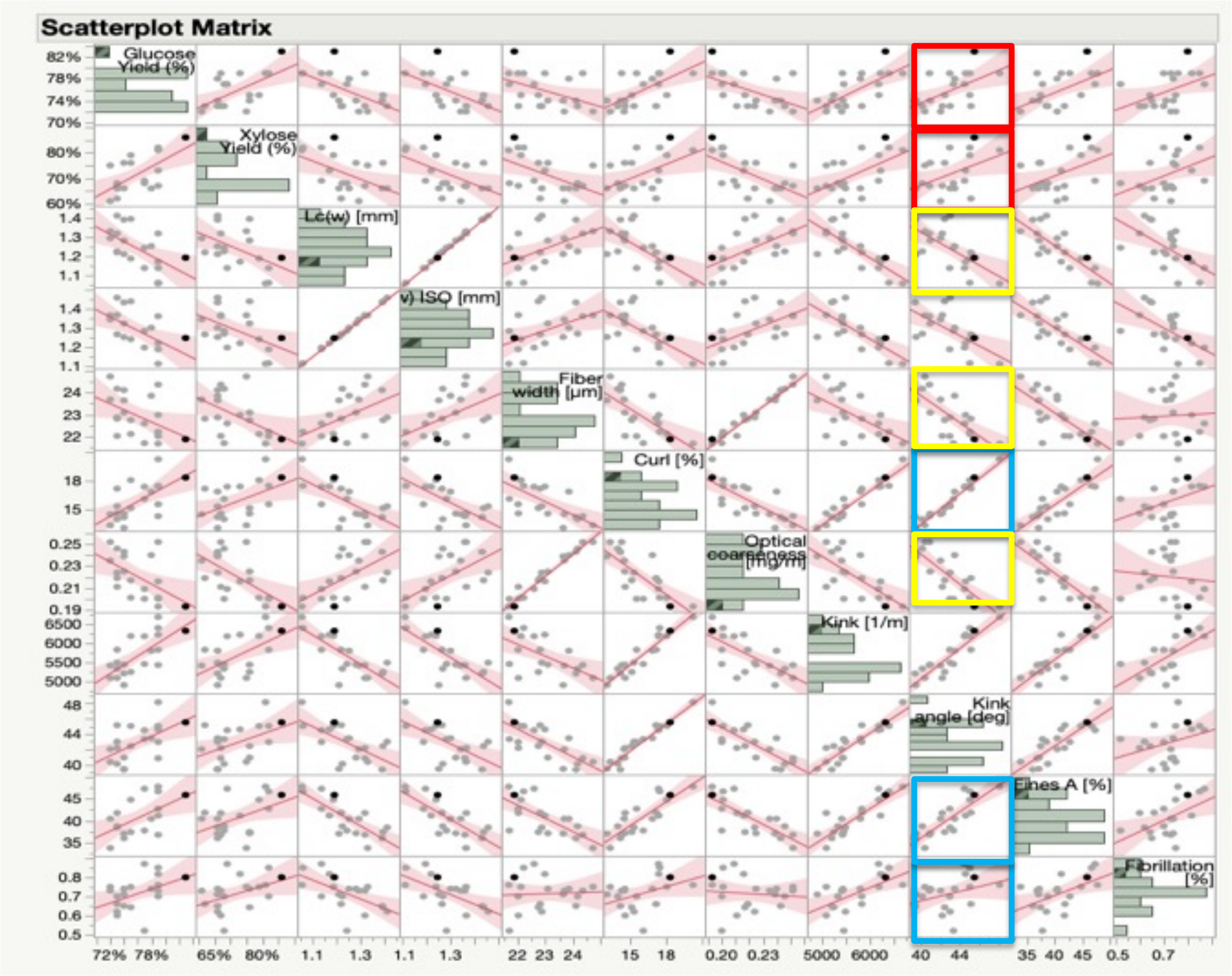




- LCA drivers: Sugar yield > energy consumption
- LCA favorite case: 10/1000 inch plate gap, 600 rpm rotational speed, and 18034A plate design

PO7: Fiber Properties and Sugar Yields

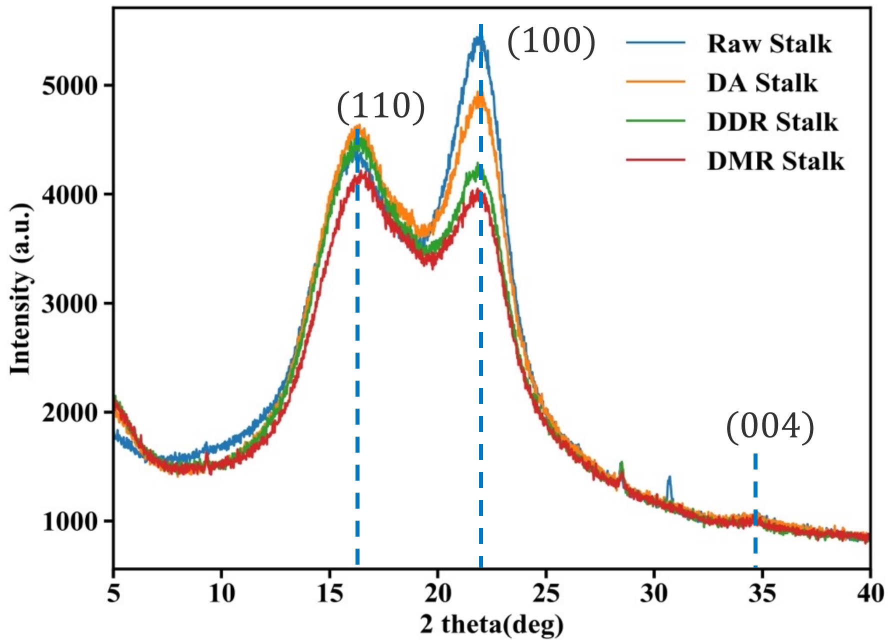


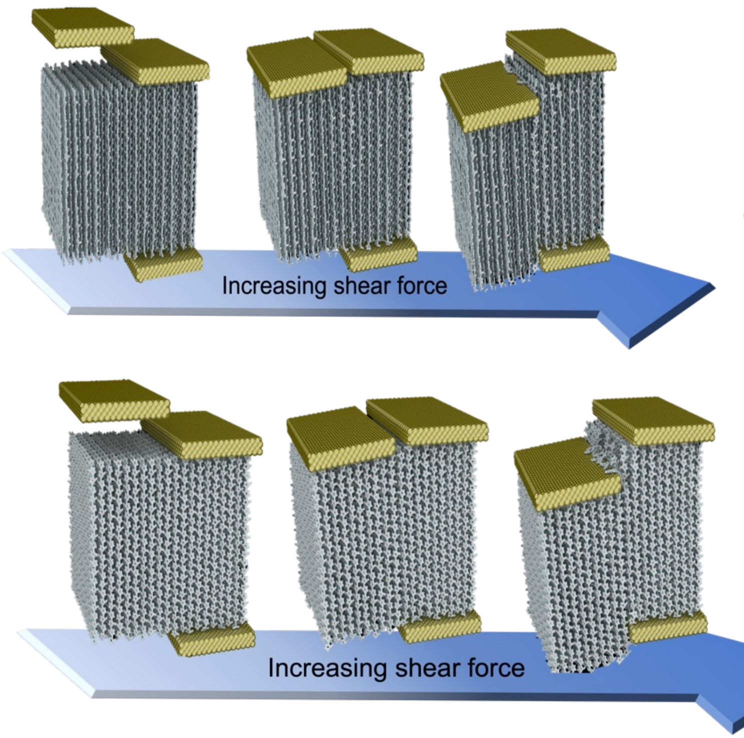


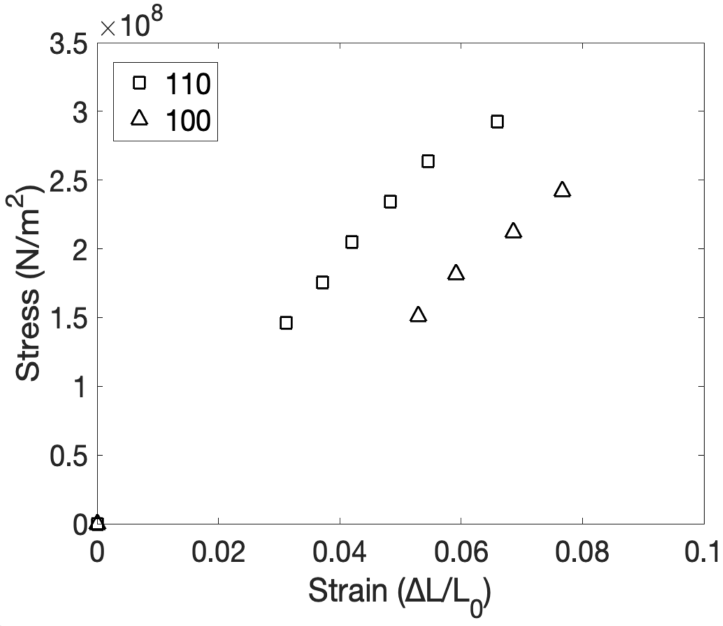
Kink reflects the damage level of the fiber

- + correlated to curls/fines/fibrillations
- - correlated to coarseness/fiber width/length
- + correlated to glucose and xylose yield (70% correlations)

PO8: Disk Refining Mechanism





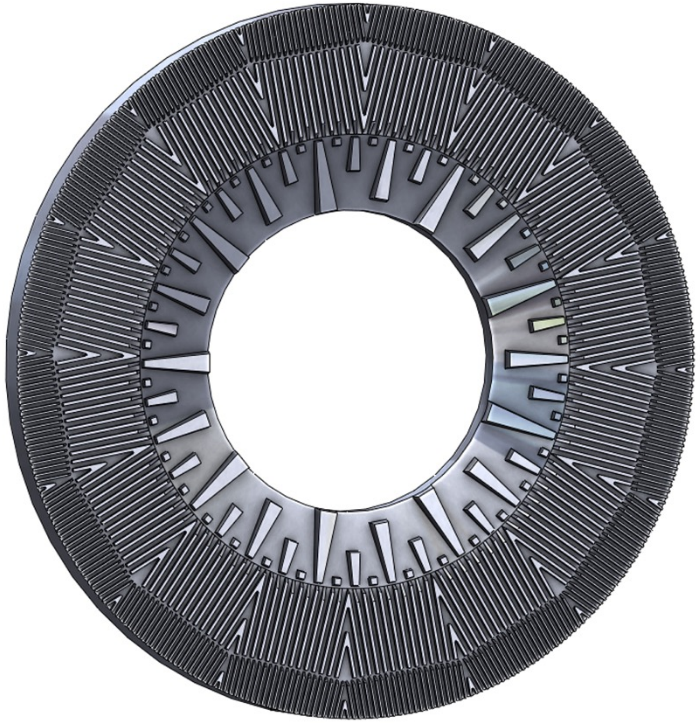


- XRD results showed mechanical fracture of cellulose along the 100 crystal planes is thermodynamically favored over fracture along the 110 planes
- Molecular dynamics simulation shows that 110 face has higher modulus and higher stress and strain to failure than 100 face

System	Modulus (GN)	Stress to failure (GN)	Strain to failure
110	4.597	0.322	0.082
100	3.118	0.242	0.077

Credits to Megan Crowley, Peter Ciesielski, Lintao Bu

Moving Forward: Scaling up to 22” Disk Refiner



- We paused the project activity in FY 22 and FY23 due to the delayed installation of the 22” disk refiner
- End of project milestone (FY24 Q4): Develop a CFD model to predict the refining energy of one set of refiner plates for 22” disk refiner and show less than 15% difference with experimental measurement

Project Impact

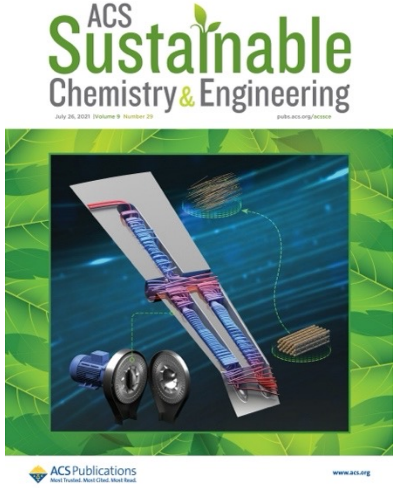
This project supports BETO’s strategic goal to :

- Decarbonize the **transportation sector** by reducing the energy consumptions during the production of sustainable aviation fuel from terrestrial biomass. (Reduce GHG in sugar production)
- Decarbonize the **industrial sector** by developing cost and energy -effective processes utilizing biomass and waste resources. (Reduce refining energy for biofuel, biochemicals and potentially pulp production)
- The optimized refining conditions and plate geometries will inform SAFFiRE Project to construct the 10 tonne/day DMR pilot plant.

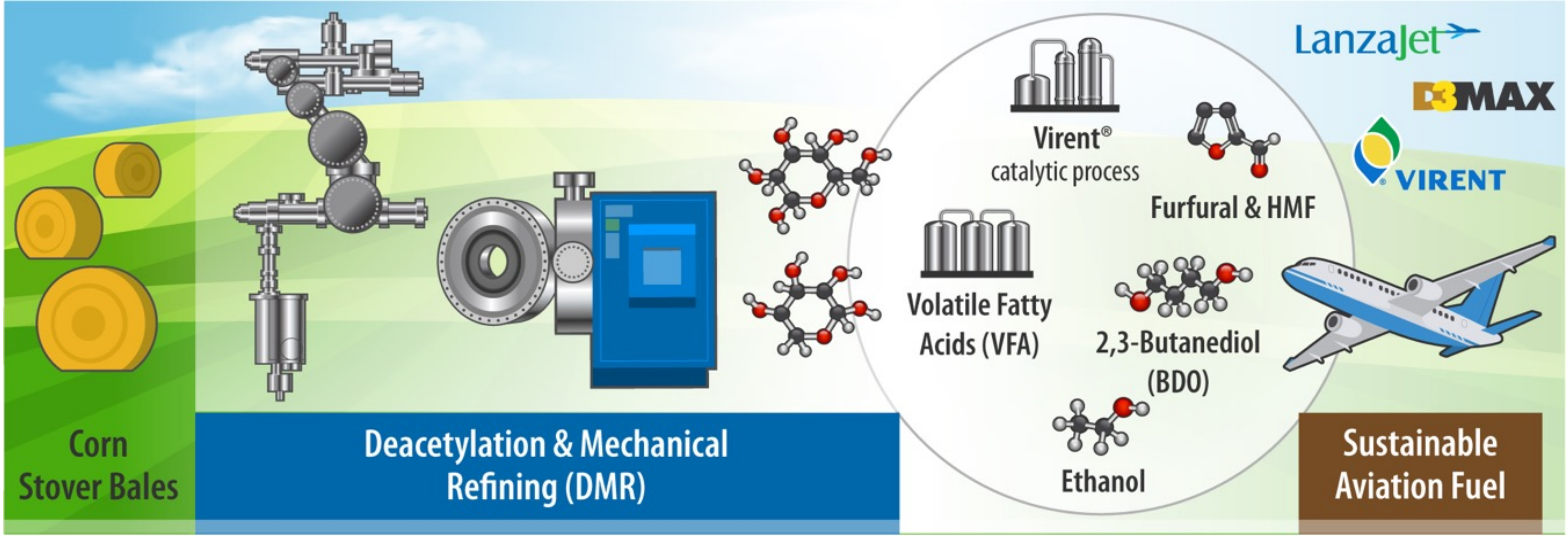
Publications:

*1. Li, Yudong, David A. Sievers, and Xiaowen Chen. "Modeling the Disc Refining of Lignocellulosic Biomass toward Reduced Biofuel Production Cost and Greenhouse Gas Emissions: Energy Consumption Prediction and Validation." **ACS Sustainable Chemistry & Engineering** (2021).*

2. Yudong, Li, Ryan Davis, David Sievers, and Xiaowen Chen. “Reducing environmental impacts of the disc refining process for the lignocellulosic biofuel industry”, Manuscript in preparation.



DMR Process as a Clean Sugar Platform



BETO relevance

- More robust and reliable compared to dilute acid pretreatment
- Produces highly fermentable cellulosic sugars at 0.20-0.25 cents/lb
- Reduces GHG emissions and increases revenue for corn EtOH plants
- DMR sugar is the platform chemical for SAF production via 2,3 BDO/ Ethanol, VFA, etc.
- By unlocking the SAF production from 150 million tons of corn stover/year, DMR process could produces > 10 billion gallons of SAF from corn stover sugars.

Summary

- A high-fidelity model developed based on NREL's 12-inch disc-refiner. The model accurately predicted energy consumption at different conditions.
- Refining energy decreases with rotational speed decrease and plate gap increase.
- Sugar yields and MSSP decrease with plate gap increase.
- Under the condition used in current study, sugar yields remains the same with rotational speed change. However, rotational speed can dramatically affect power consumptions. MSSP decrease dramatically with rotational speed decrease
- Refiner plate geometric designs affect both power consumptions and sugar yields. Based on TEA, plate geometries with high sugar yields result in low MSSP.
- By optimizing the plate geometric design and refining conditions, we will be able to reduce refining energy consumptions which will lead to reduced MSSP and reduced GHG emissions.

Quad Chart Overview

Timeline

- Start date: 10/01/2019
- End date: 9/30/2022 (delayed to 9/30/2024)

	FY22 Costed	Total Award
DOE Funding	*$100,000* *($200,000 left)*	$750,000
Project Cost Share*		

TRL at Project Start: 3
TRL at Project End: 4

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

Project Partners*

- Andritz

Thank you!

www.nrel.gov

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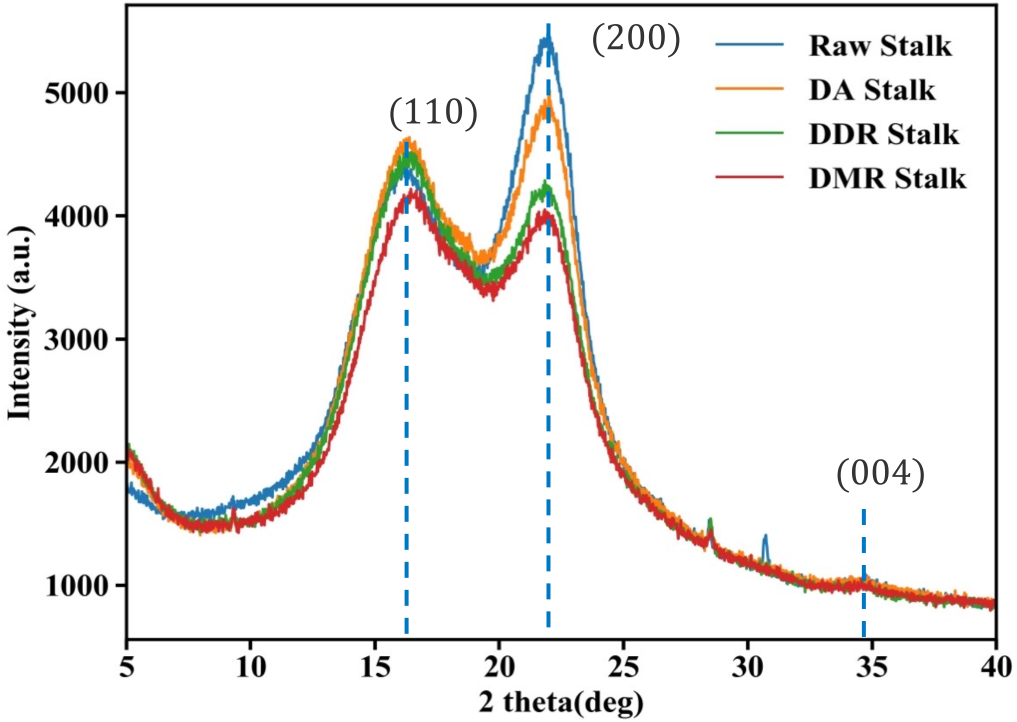
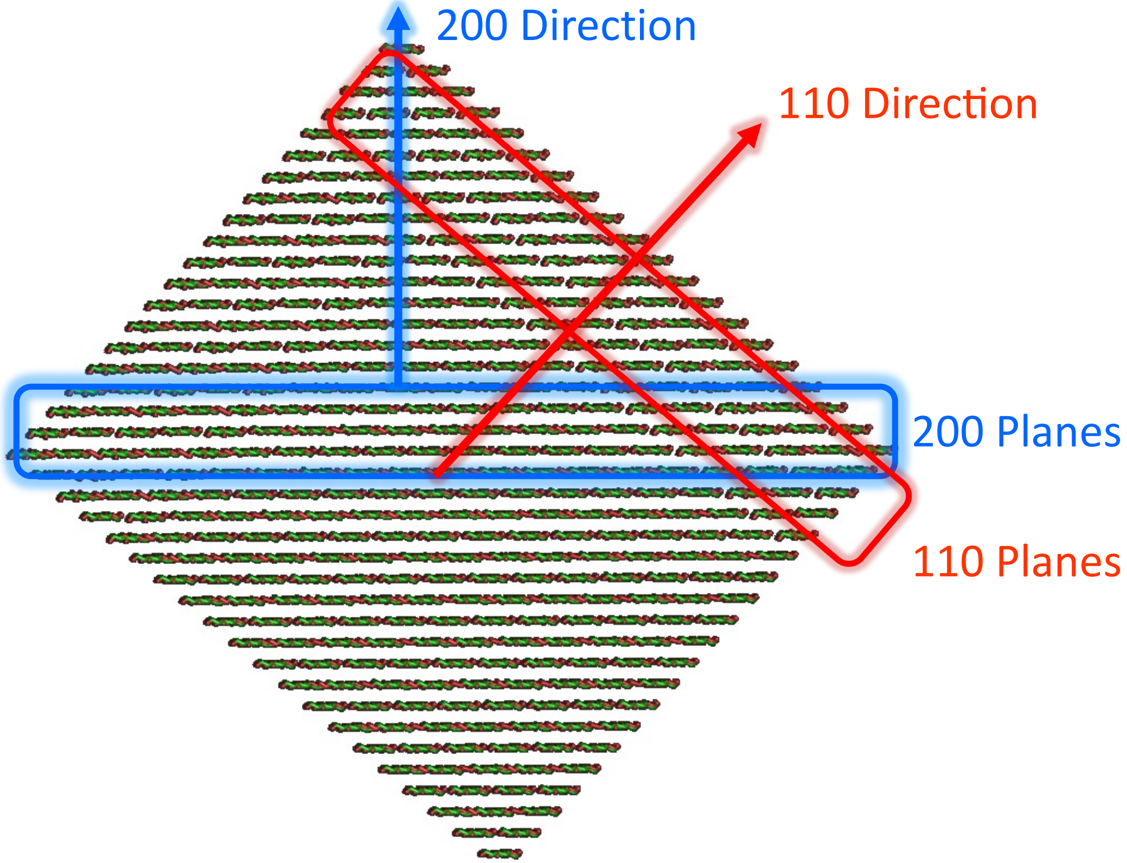
NREL

Transforming ENERGY

Why Disk Refining?





- X-ray reflection intensity from the 200 planes are disproportionately attenuated as pretreatment progresses
- Fragmentation patterns that disrupt stacking of 200 planes are more frequent than those that disrupt the 110 direction

Hypothesis: Mechanical fracture of cellulose along the 200 crystal planes is thermodynamically favored over fracture along the 110 planes