Co-Optimization of
Fuels & Engines

# Fuel Property-Informed Process Design for the Direct Catalytic Conversion of Cellulosics

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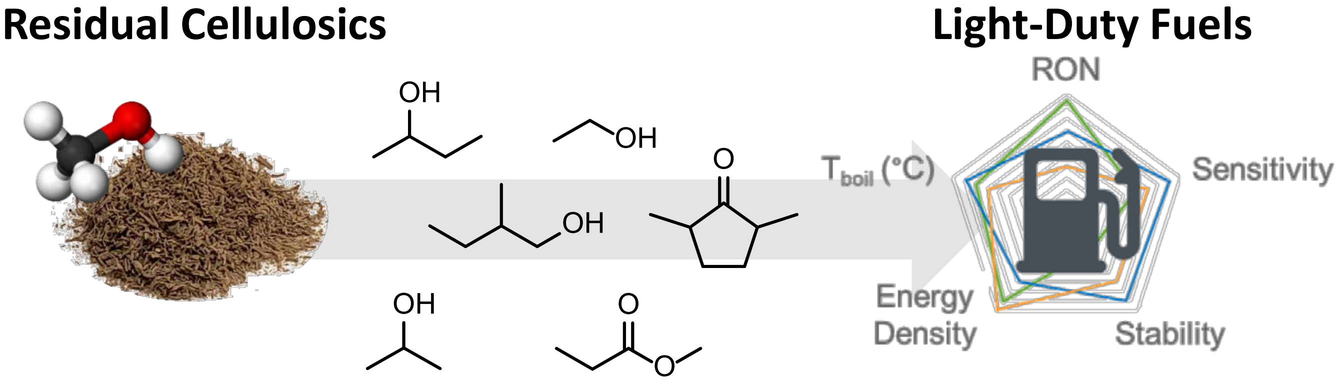
August 20th, 2020


U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

American Chemical Society
Fall 2020 Virtual Meeting & Expo

# Motivation & Background



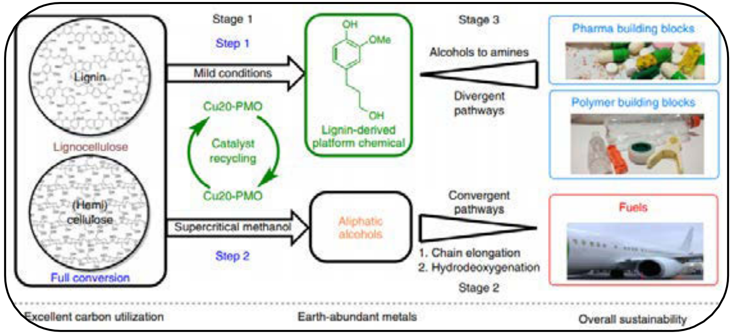

**Goal: Development of a light-duty fuel using fuel property-informed catalytic/process development**



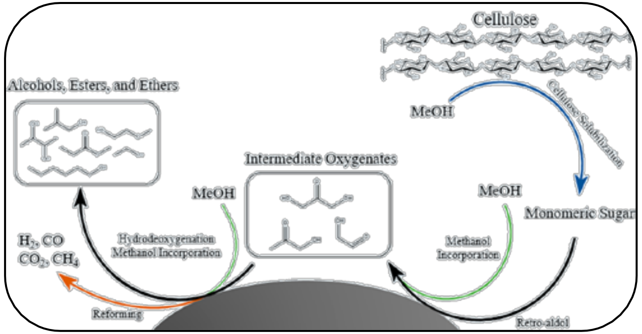
Nguyen et al. (2020), in preparation

# Motivation & Background

## **Direct Catalytic Conversion of Cellulosics (DC3)**, a History




*Nature Catalysis* **2018** 1**,** 82–92




*ACS Sustainable Chemistry & Engineering* **2018** *6* (3), 4330-4344

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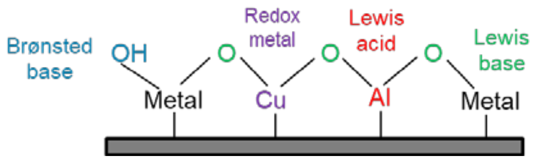
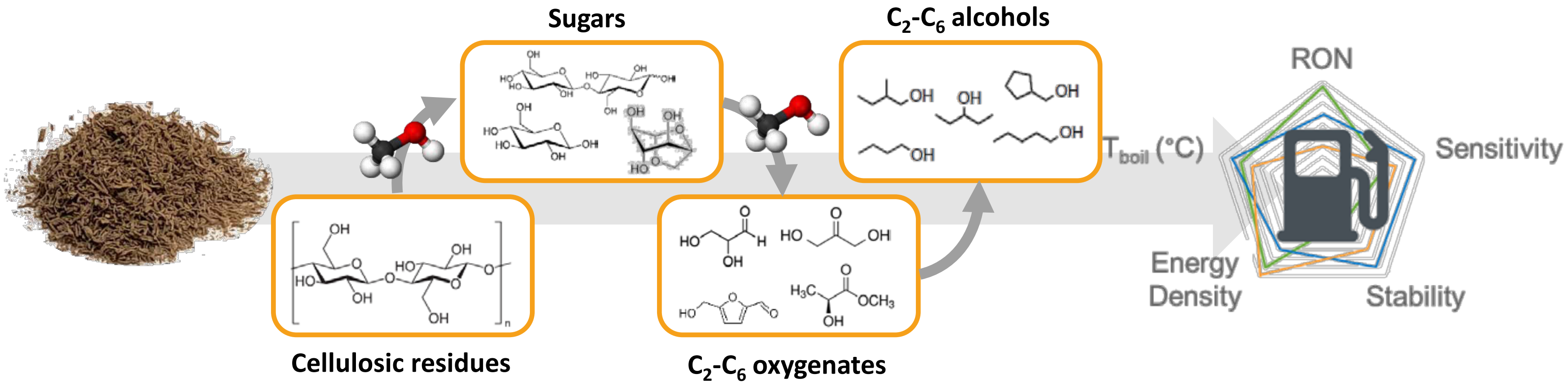
## **Is there a fuel application?**

# Approach




**What is a "good" fuel?**



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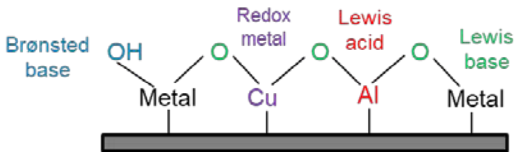
# Approach

## Process Tunability

The product slate changes depending on reaction conditions, catalyst design, and separation strategy

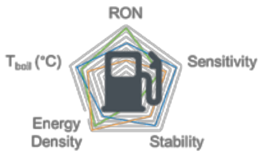



### Product Analysis

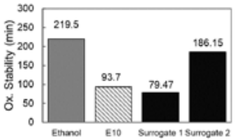

### Process Tuning

## Fuel Design

Significant unknowns regarding fuel properties can be revealed using surrogate and product fuel testing




### Surrogate Testing




### Surrogate Reformulation



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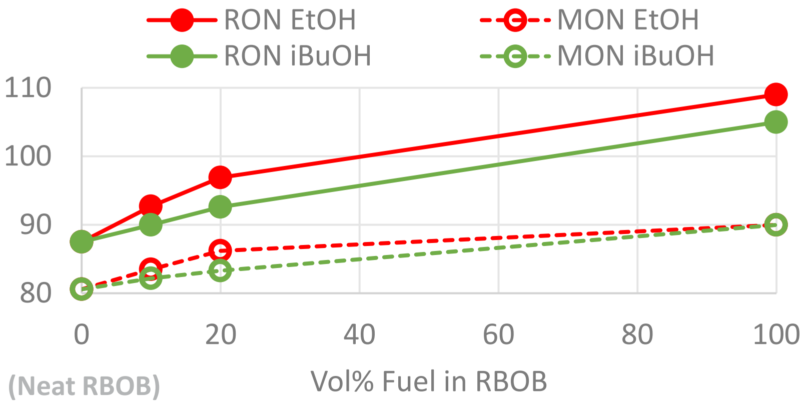
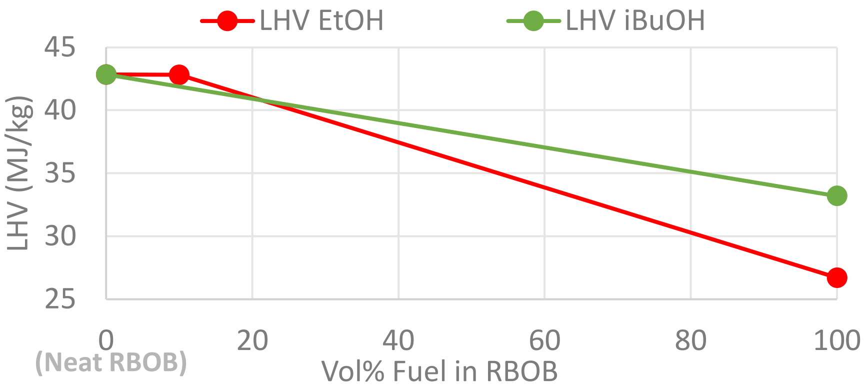
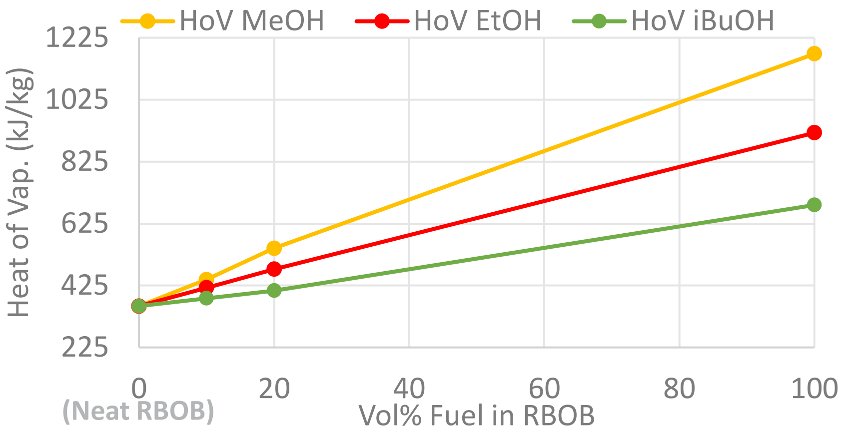
# Approach: test one blend level in RBOB



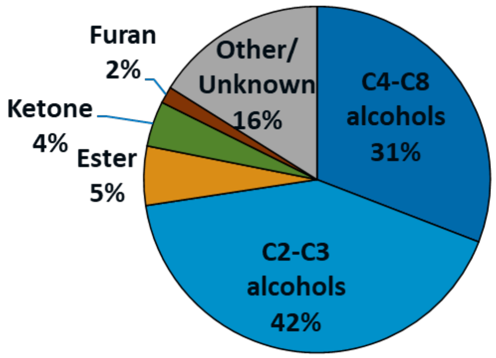



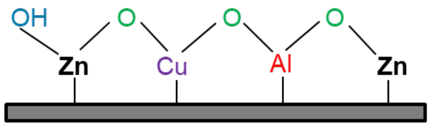




McCormick et al., 2017; Co-Optima Fuels Database

# Surrogate Experiments

## Product Composition




| Fuel Property | Direction of Improvement | Neat EtOH | CuZnAl Surrogate | |
|---|---|---|---|---|
| | | | Top 20 | Alcohols from Top 20 |
| LHV (MJ/kg) | ↑ | 21.1 | 29.93 | 30.63 |
| Density (g/mL) | – | 0.789 | 0.823 | 0.806 |
| RON | ↑ | 109 | 109.9 | 109.6 |
| S | ↑ | 19 | > 10 | > 10 |
| HoV (kJ/kg ) | ↑ | 839 | 659 | 723 |
| Cloud Pt. (°C) | ↓ | -114 | -65.40 | < -75 |
| T90 (°C) | ↓ | 78.37 | 165 | 165 |
| Ox. Stability (min) | ↑ | 219.52 | 79.47 | 186.15 |



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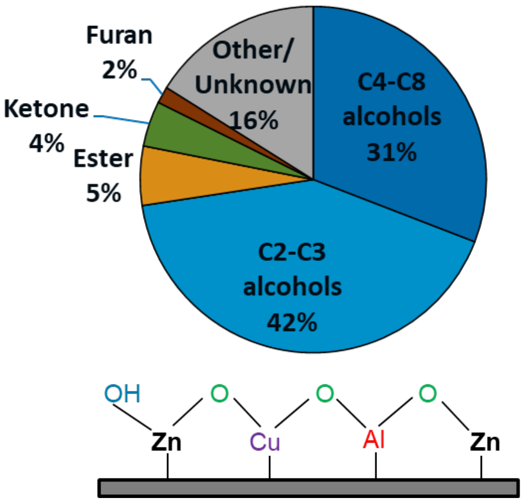
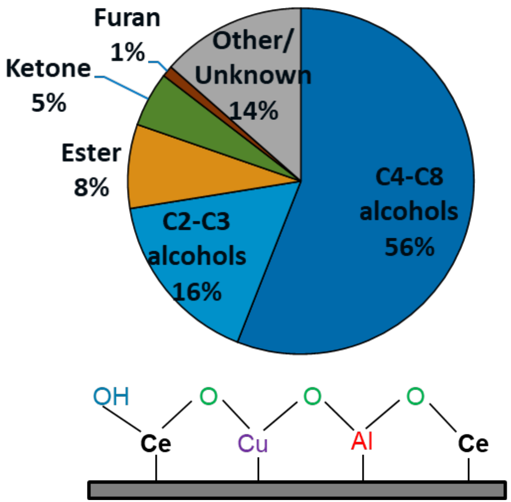
# Surrogate Experiments

## CuZnAl Product Composition




**Process Advancement**

## CuCeAl Product Composition



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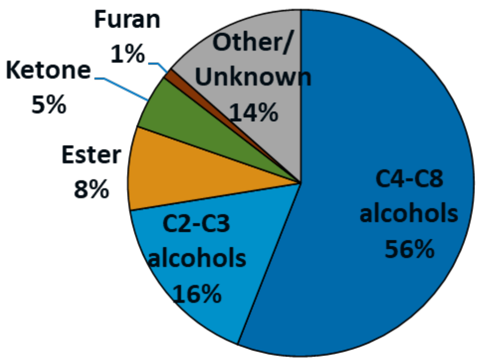
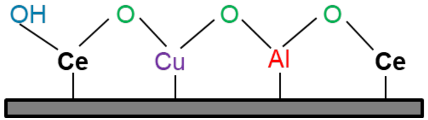
# Questions

- How do the fuel properties fare upon blending into a base fuel?
- What is the impact of unreacted methanol in the product?
- What parameters require attention while attempting scale-up of the real bioderived product?

Reformulated DC3 Product



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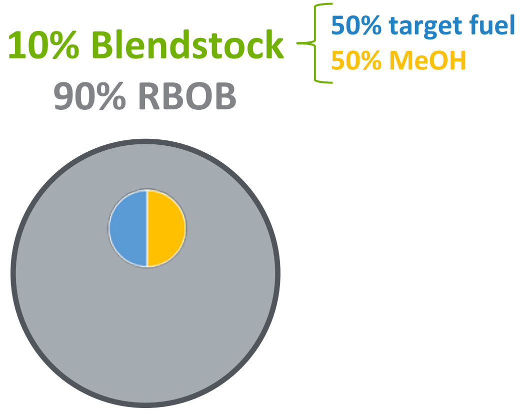
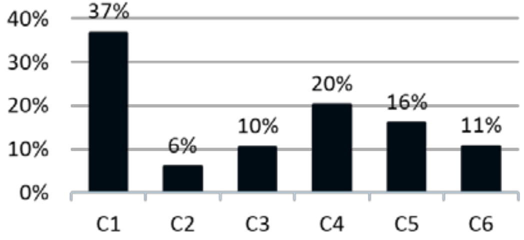
# Questions

- How do the fuel properties fare upon blending into a base fuel?
  → 10 vol % blends in RBOB
- What is the impact of unreacted methanol in the product?
  → Incorporated MeOH to blend limit
- What parameters require attention while attempting scale-up of the real bioderived product?



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# Questions

- How do the fuel properties fare upon blending into a base fuel?
  ➔ 10 vol % blends in RBOB
- What is the impact of unreacted methanol in the product?
  ➔ Incorporated MeOH to blend limit
- What parameters require attention while attempting scale-up of the real bioderived product?
  ➔ Preliminary biofuel characterization



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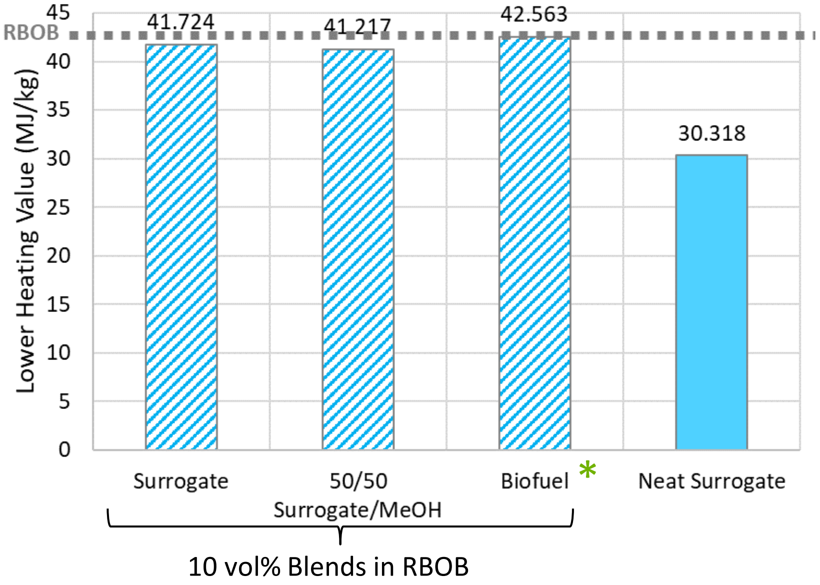
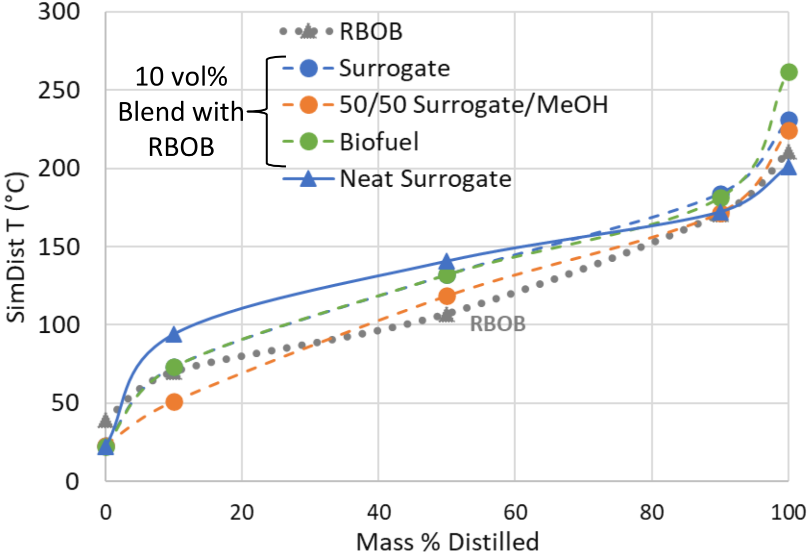
# Fuel Properties

## Energy Density




## Simulated Distillation




*Preliminary sample



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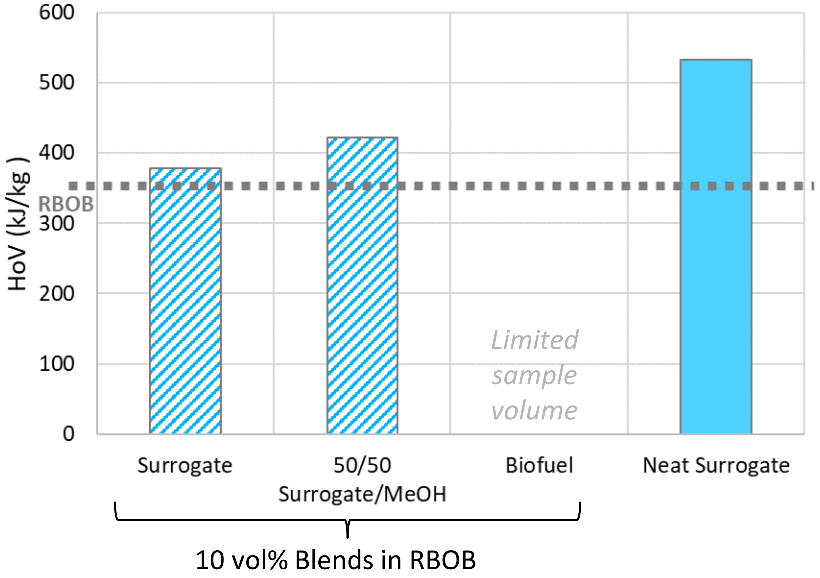
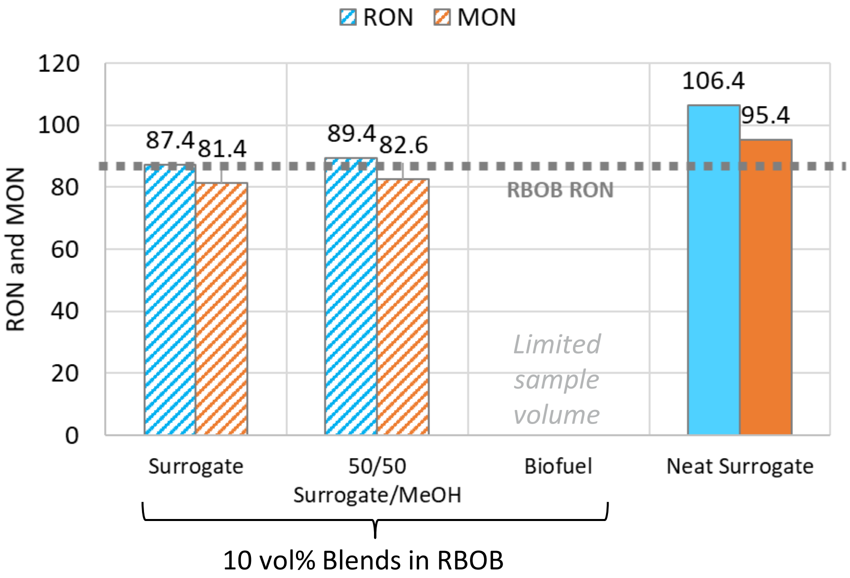
# Fuel Properties

## Heat of Vaporization




## Ignition Characteristics



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# Scaleup Considerations

- Can (or should) selectivity be increased?
- How can we test and utilize commercial water removal techniques at the bench scale?

- What is the optimal BOB or base fuel?
- How high can we push the product blend level?

**Process Tunability** ⟷ **Fuel Design**

- How should we treat MeOH, considering:
    - Impacts on fuel properties and product quality?
    - Implications of recycle?
    - Unit operation costs?



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# Conclusions

## Ongoing Work

- Water removal studies
- MeOH recycle experiments
- Scaled processing using continuous flow reactors
- Preliminary design of scaled distillation units
- Preliminary technoeconomic analyses

## Summary

- An iterative structure-property-approach process resulted in measurable process improvements through fuel considerations
- Confirmed blend compatibility of dry product in RBOB
- Blend testing using surrogates suggested promising fuel properties of the real product, even with residual MeOH
- Promising preliminary testing of real product


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# Acknowledgements

Lead: Hannah Nguyen

Daniela Stück

Stephen M. Tifft

PI: Derek R. Vardon

**Many thanks to**

- Cameron Hays
- Gina Chupka
- Earl Christensen
- Jon Luecke
- Bob McCormick

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This work was authored by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. This research was conducted as part of the Co-Optimization of Fuels & Engines (Co-Optima) project. Funding provided by the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Bioenergy Technologies Office, and the Vehicle Technologies Office. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.