



Direct Catalytic Conversion of Cellulosics (DC3)

DOE Bioenergy Technologies Office
2019 Peer Review

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ENERGY

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& RENEWABLE ENERGY

BIOENERGY TECHNOLOGIES OFFICE

Direct Catalytic Conversion of Cellulosics (DC3)

Background, Goal, and Outcome



ChemCatBio Goal: Accelerate the development of catalysts and related technologies for the commercialization of biomass-derived fuels and chemicals

❖ DC3 Background

Conversion processes are needed to valorize both the cellulosic and lignin fractions of biomass. Lignin monomers can be selectively removed by “Lignin First” solvolysis for upgrading. However, compatible processes are still needed for the residual cellulosics.

❖ DC3 Goal

The goal of DC3 is (i) develop a semi-continuous solvolysis + catalysis process to upgrade residual cellulosics from delignified biomass, and (ii) demonstrate the resulting oxygenates are suitable as a biofuel.

❖ DC3 Outcome

This project will advance a new conversion process within the BETO portfolio that is (i) fully compatible with “Lignin First” upgrading, and (ii) expands the slate of fuels and chemicals derived from cellulosics.

Quad Chart



Timeline

- **Project start date:** Oct 1, 2018
- **Project end date:** Sept 30, 2020
- **Percent complete:** 25%

	Total Costs Pre FY17*	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19- End)
DOE Funded	\$0k	\$0k	\$134k	\$402k

BETO Projects: Lignin First, Lignin Utilization, Co-Optima, Catalytic Upgrading of Biochemical Intermediates
Universities: University of Wisconsin (George Huber)

Barriers Addressed

- Ot-B. Cost of Production**
- Ct-F. Increasing Yield from Catalytic Processes**

Objectives

- Aim 1.** Deploy a semi-continuous solvolysis + catalysis process for converting delignified woody biomass to mixed aliphatic alcohols
- Aim 2.** Evaluate multi-functional catalysts for tailoring the alcohol production distribution
- Aim 3.** Produce DC3 biofuel to validate the fuel properties and target >15% MFSP savings compared to state-of-the-art

End of Project Goal

Establish a semi-continuous solvolysis + catalysis approach to (i) generate oxygenated fuels with suitable properties from delignified woody biomass, and (ii) determine metrics necessary to meet a <\$3.00/GGE based on integrated TEA with “Lignin First” valorization

1 - Project Overview

Enable an integrated approach for “Lignin First” upgrading

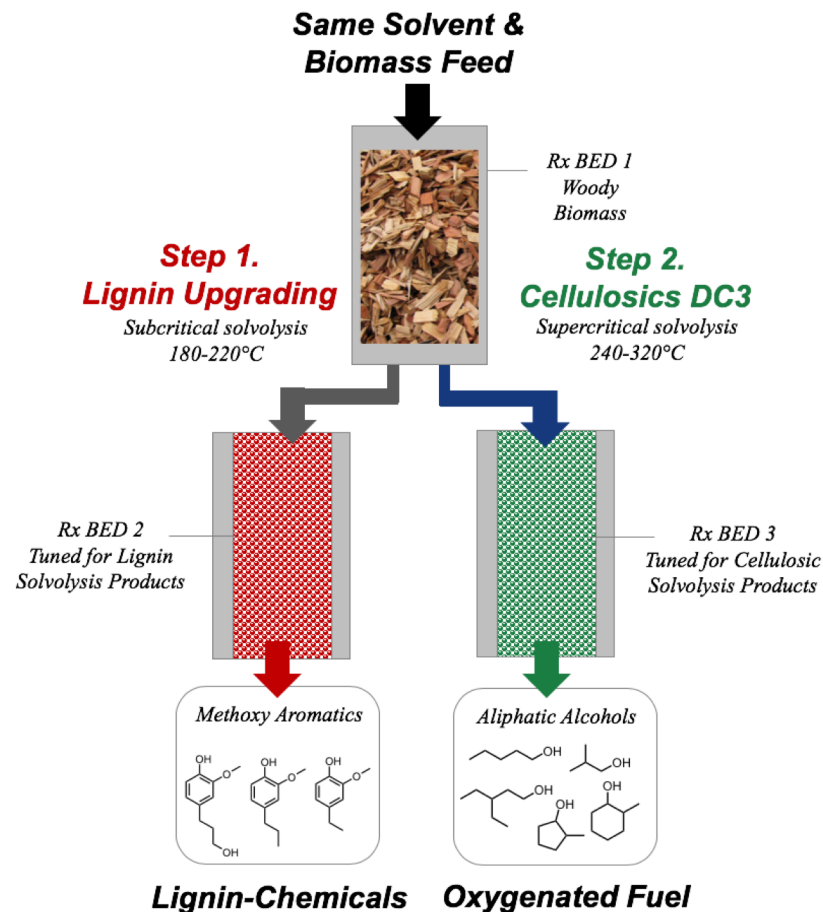


Background on “Lignin First”

- ✓ Lignin monomers initially removed by subcritical solvolysis with methanol
- ✓ After solvolysis, lignin monomers processed with downstream catalysis for making fuels and/or chemicals

Integration with DC3

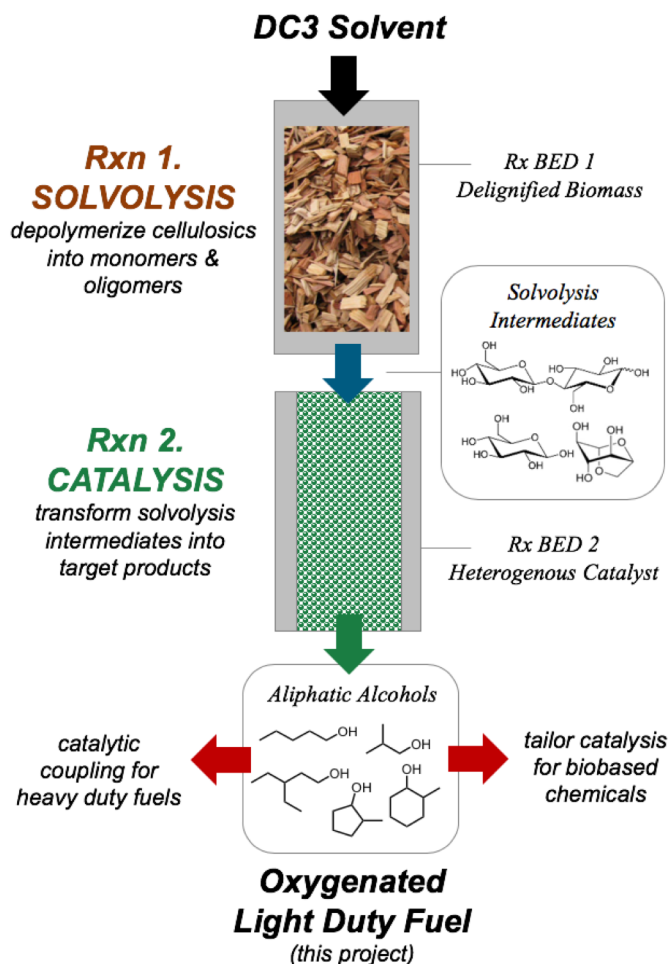
- ✓ Residual cellulosics can be fully solubilized using same solvent under supercritical conditions
- ✓ Cellulosic monomers can be processed over their own tailored catalyst bed for making fuels and/or chemicals



DC3 integrates with “Lignin First” upgrading via solvolysis + catalysis

1 - Project Overview

Motivation and key questions remaining for DC3



Motivation for DC3

- ✓ DC3 can convert delignified woody biomass, as well as waste cellulose, into energy dense liquid oxygenates
- ✓ Provides opportunity to target gasoline, precursors for diesel, and/or chemicals

Key Questions for DC3

- ✓ Need to better understand feedstock and interface with “Lignin First”
- ✓ Need to assess (i) DC3 oxygenate fuel properties, (ii) ability to steer product distribution, and (iii) overall economics

DC3 utilizes solvolysis + catalysis to upgrade cellulose

1 - Project Overview

Prior history and proposed processing approach to advance DC3



History of DC3 Batch Rxn



*Batch Rxn
combines*

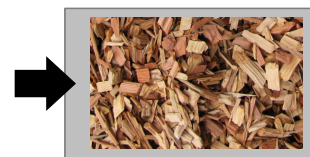
**SOLVOLYSIS
& CATALYSIS**

- ✓ Challenge to scale low-cost, high-volume batch processes
- ✓ Relies on contacting solid biomass w/solid catalyst initially
- ✓ Cannot decouple solvolysis and catalysis reaction steps

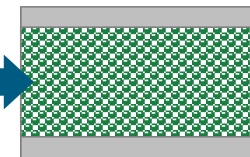
Move to Semi-Continuous

Semi-continuous decouples rxn

**Step 1.
SOLVOLYSIS**



**Step 2.
CATALYSIS**

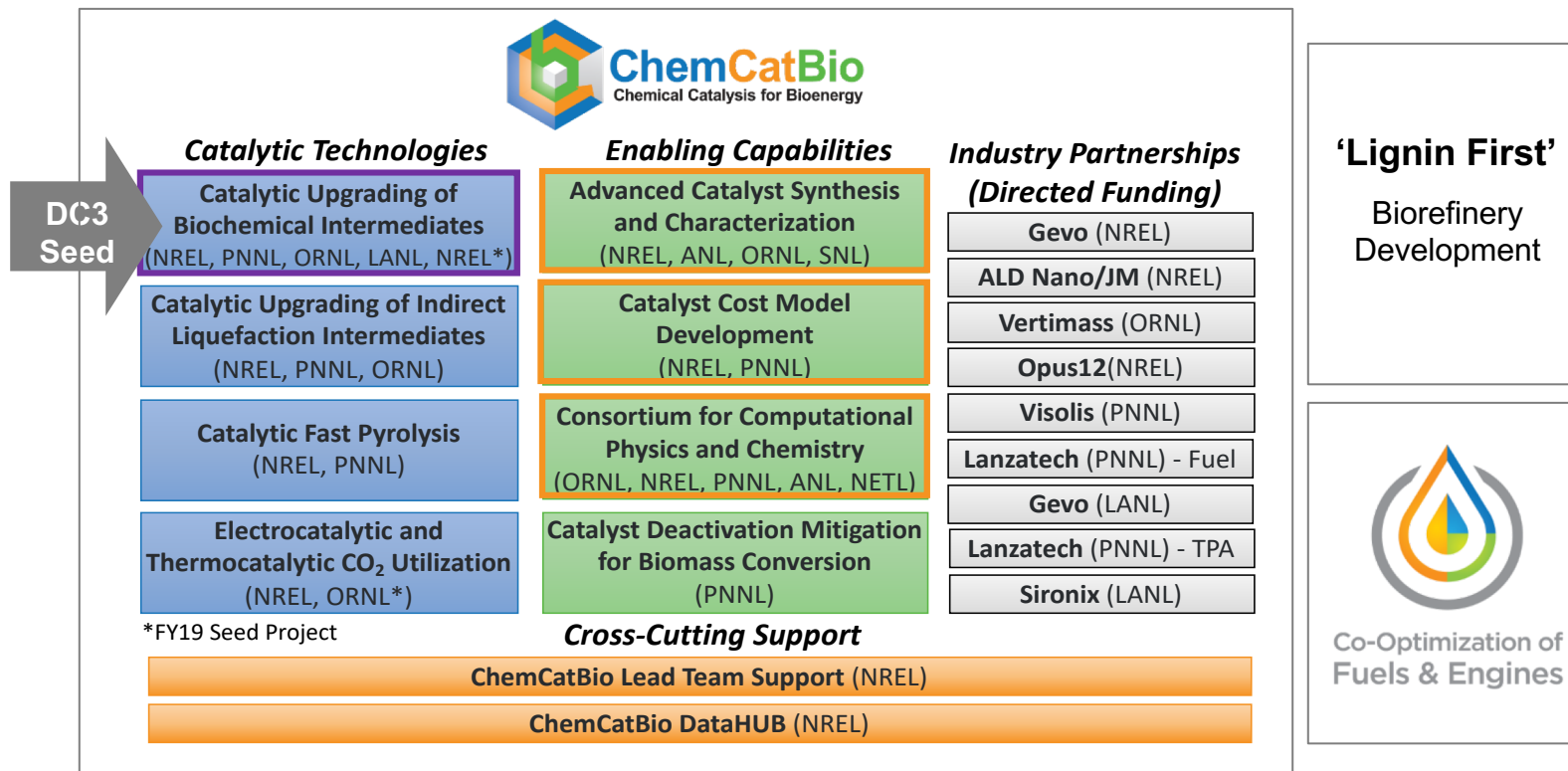


- ✓ Potential for simplified flow through solvent processing
- ✓ Only react soluble monomers & oligomers over solid catalyst
- ✓ Independently tune solvolysis and catalysis reaction steps

DC3 project will extend prior batch studies to semi-continuous

2 - Approach (Management)

How DC3 fits within CCB and interfaces with the BETO portfolio



- Work with ChemCatBio on catalyst cost modeling (CCM) and advanced characterization (ACSC)
- Coordinate with 'Lignin First' on delignified biomass and solvent selection
- Collaborate with Co-Optima on leveraging latest fuel property tools

DC3 is a new start seed project within ChemCatBio

2 - Approach (Management)

Project team with management best practices



Project Team Roles and Current Collaborations



Derek Vardon, PI

NREL DC3 Team: *Hannah Nguyen, Nick Cleveland*

NREL Collaborators:

Lignin First - Gregg Beckham

CatCostModel- Fred Baddour

Economic Analysis - Mary Bidy

ACSC - Susan Habas

External Collaborators:

Catalysis + Solvolysis - George Huber, University of Wisc.

DC3 Project Communication & Coordination

1) Biweekly technical planning meetings with core team

- Recap accomplishments, assign action items, review objectives

2) Quarterly planning meetings with DC3 collaborators

- Discuss alignment, review progress, coordinate next steps

Utilize best management practices and build collaborations

2 - Approach (Technical)

Major project goals and research approach



DC3 for Upgrading Residual Cellulosics

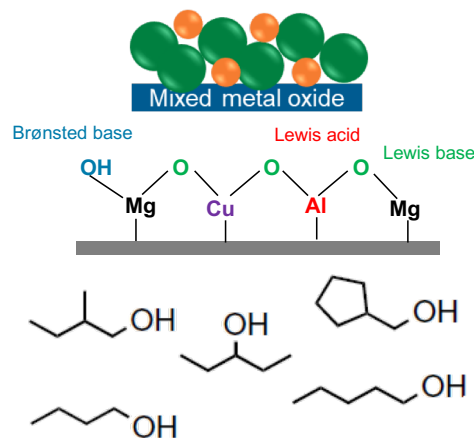
Process Development

Deploy a semi-continuous DC3 process for converting delignified woody biomass to mixed aliphatic alcohols



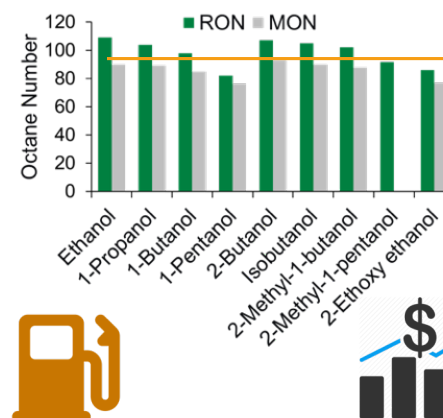
Catalyst Design

Evaluate multi-functional catalysts for aliphatic alcohol production and solvent reforming



Biofuel Evaluation

Produce DC3 biofuel to validate the fuel properties and >15% MFSP savings compared to state-of-the-art



Span process development, catalyst design, and biofuel R&D

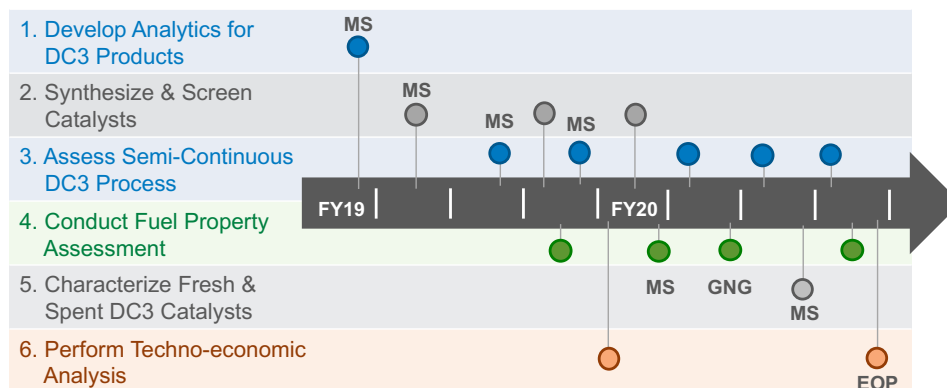
2 - Approach (Technical)

Well-defined milestones and strategies to address risk



Potential Risk	Mitigation Strategy
<ul style="list-style-type: none">✓ Rapid catalyst deactivation during DC3 biomass processing✓ Poor oxygenate recovery following conversion✓ In-sufficient information on fuel properties of oxygenate blendstock	<ul style="list-style-type: none">✓ Evaluate regeneration schemes, as well as biomass pre-wash✓ Assess separation techniques (distillation, extraction)✓ Collaborate with Co-Optima for latest fuel property prediction tools

Project Milestones (MS) with Go-No/Go (GNG)



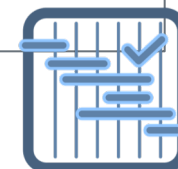
Progress measurable with risk mitigation in place

2 - Approach (Technical)

Critical success factors, challenges, and key activities



Critical Success Factor	Challenge to Overcome	Activity to Address
Transition from batch to semi-continuous operation	<ul style="list-style-type: none">Lack of published dataDiffering performance	Deploy semi-continuous DC3 reactor as major focus in FY19
Achieve high yields of oxygenates with minimum solvent loss	<ul style="list-style-type: none">Excess MeOH reformingLow yield of fuel target	Evaluate tunable catalyst suite with pre/post characterization
Deliver lower cost higher performing oxygenated biofuel	<ul style="list-style-type: none">Unknown fuel propertiesLow TRL for process	Conduct mid and final TEA with fuel property assessment



Project activities designed to address barriers to success

3 - Relevance

How DC3 contributes to BETO goals and objectives



Contribute to BETO Goals

Ot-B. Cost of Production

- Assess new “solvolysis + catalysis” that allows for parallel lignin valorization
- Conduct TEA to inform production costs and identify major cost drivers for follow-on R&D



Ct-F. Increase Yield from Catalytic Processes

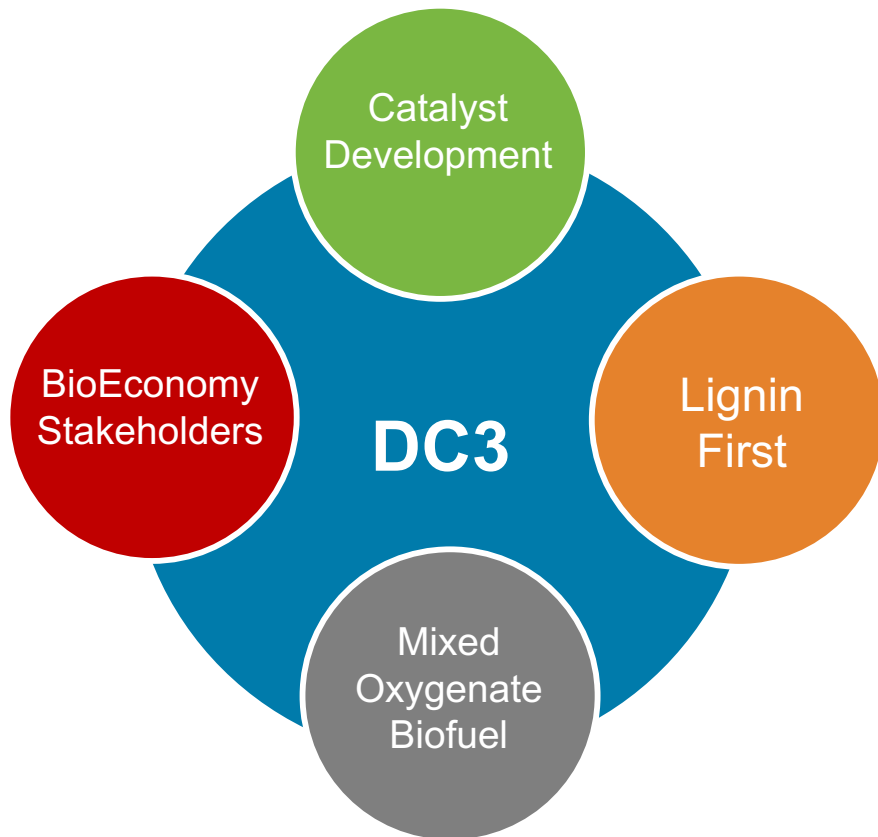
- Benchmark against commercial and literature catalysts
- Leverage fuel property tools to define targets
- Test suite of catalysts to improve target product yields



ChemCatBio Goal: Accelerate the development of catalysts & related technologies for the commercialization of biomass-derived fuels & chemicals

3 - Relevance

Potential applications, advancement in SOT, impact to viability



Impact Viability of Bioenergy

- Develop strategy with “Lignin First”
- Leverage solvolysis + catalysis to simplify unit operations for upgrading
- Demonstrate value of fuel that retains oxygen inherent to biomass

Potential DC3 Applications

- Target industries that have waste cellulosic feedstocks (pulp and paper)
- Develop tunable process to target oxygenated fuels *and* chemicals

Advancement in SOT

- Further derisk catalytic solvolysis strategies from batch to flow
- Assess catalyst tailorability and stability and resulting economics

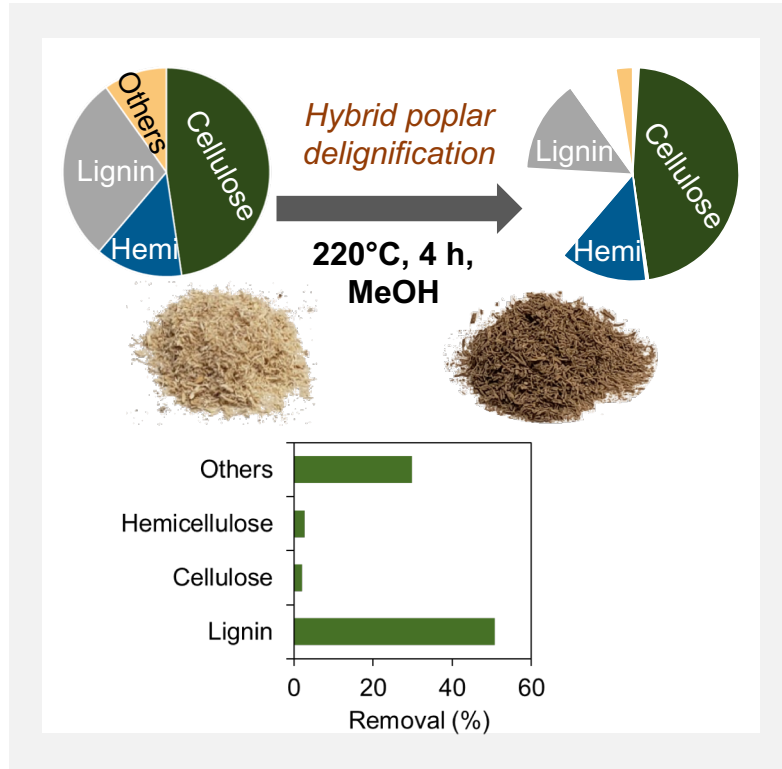
Ensure DC3 project is of high impact to biomass community

4 - Future Work



Produce and characterize delignified DC3 biomass feedstock

Research Goal: Generate delignified biomass and retain (hemi)cellulose



Planned Activities:

- Generate delignified hybrid poplar using subcritical MeOH solvolysis
- Assess feedstock composition using NREL expertise in biomass compositional analysis
- Collaborate with “Lignin First” team on lignin removal technology

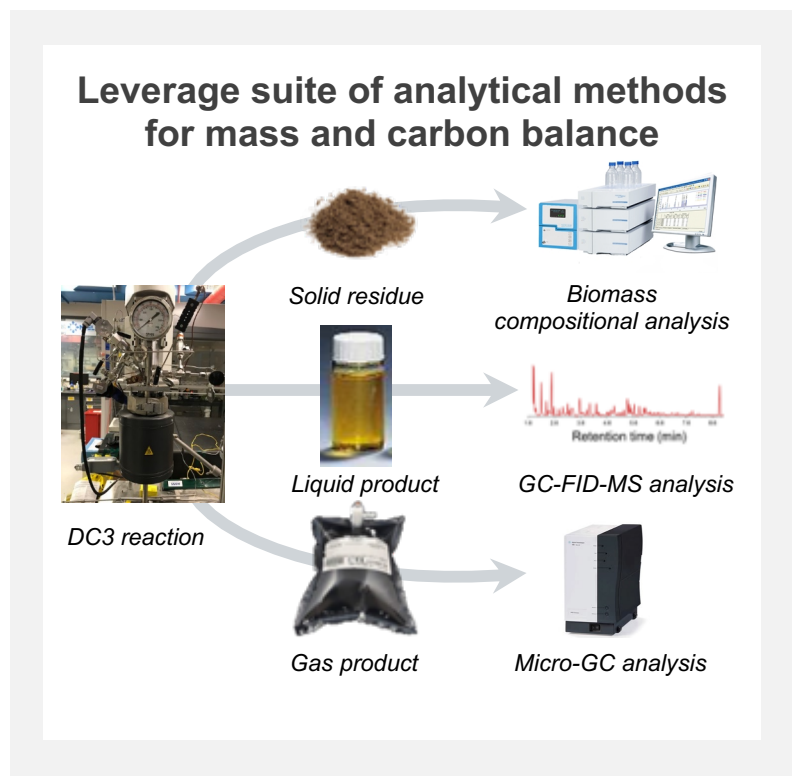
Target: Produce and analyze DC3 feedstock at the >10-gram scale

4 - Future Work

Develop analytical methods for DC3 processing



Research Goal: Quantify biomass conversion, products, and solvent



Planned Activities:

- Develop GC/LC methods to analyze composition of gas/solid/liquid products
- Quantify conversion, yield, selectivity and solvent loss
- Develop collaborations for complex product analysis via NMR and FT-ICR-MS

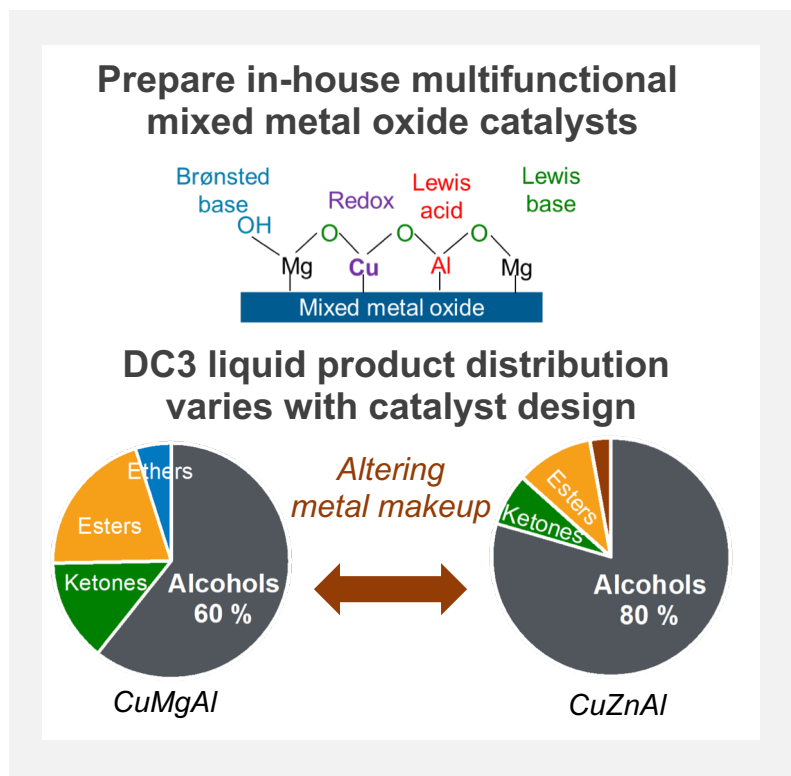
Target: Achieve gas/liquid/solid mass & C-balance with 90% closure

4 - Future Work



Tune catalyst composition for desired products and solvent retention

Research Goal: Develop tunable mixed metal oxide catalysts for DC3



Planned Activities:

- Benchmark against commercial and literature
- Evaluate tailored suite of mixed metal oxides
- Leverage ChemCatBio ACSC and Catalyst Cost Model
- Link product distribution to favorable fuel properties and/or chemical applications

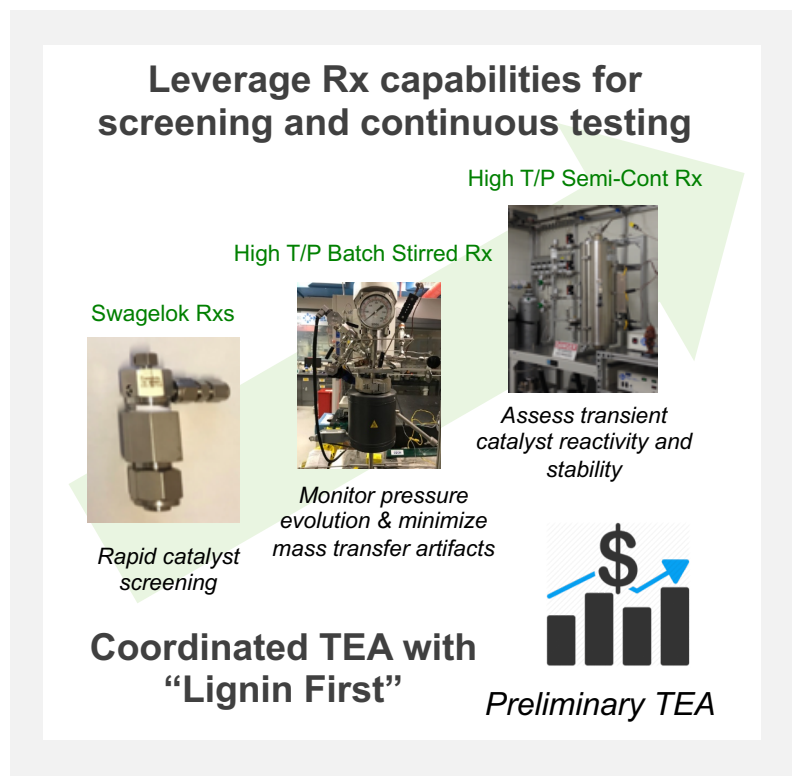
Target: Baseline against commercial and screen >8 tuned catalysts

4 - Future Work



Deploy semi-continuous DC3 process with informed TEA feedback

Research Goal: Deploy semi-continuous DC3 at 5-g biomass scale



Planned Activities:

- Investigate DC3 performance in batch and flow
- Utilize a high T/P flow reactor for semi-continuous DC3
- Investigate sustained activity for down-selected catalysts
- Leverage early-stage TEA to inform process parameters

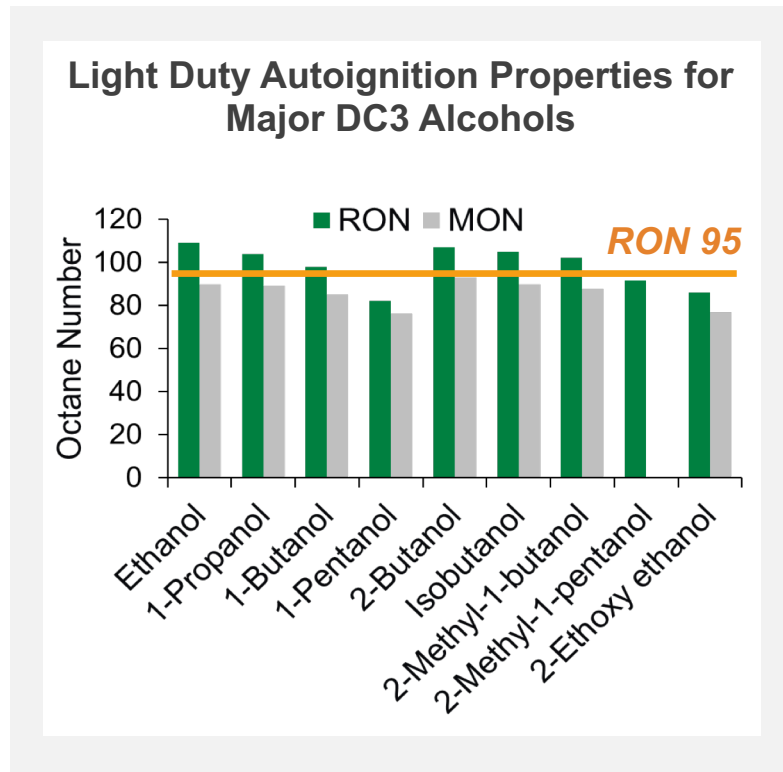
Target: Achieve semi-continuous >50% C-yield to aliphatic alcohols

4 - Future Work

Evaluate fuel properties of DC3 aliphatic alcohols



Research Goal: Set DC3 conversion targets based on fuel properties



Planned Activities:

- Leverage Co-Optima fuel property tools to set conversion targets
- Tune catalyst & process conditions to generate desirable oxygenate fuel
- Generate >20 mL of DC3 oxygenates and measure fuel properties as 20% blend

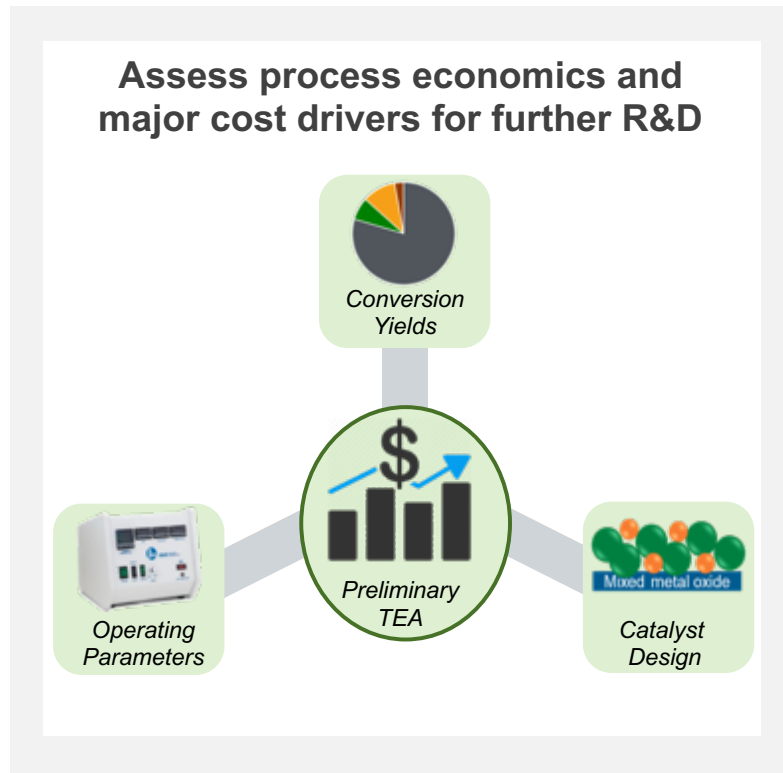
Target: Demonstrate suitable DC3 fuel properties at 20% blend level

4 - Future Work



Perform integrated TEA analysis to inform process development

Research Goal: Understand major process cost drivers for DC3



Planned Activities:

- Provide process parameters for TEA and plan R&D to address major cost drivers
- Utilize Catalyst Cost Model to inform catalyst down-selection
- Update cost models at end of project with “Lignin First” to show pathway to <\$3/GGE

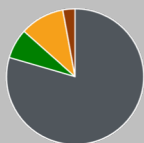
Target: Show pathway to <\$3.00/GGE fuel with DC3 & Lignin First

4 - Future Work

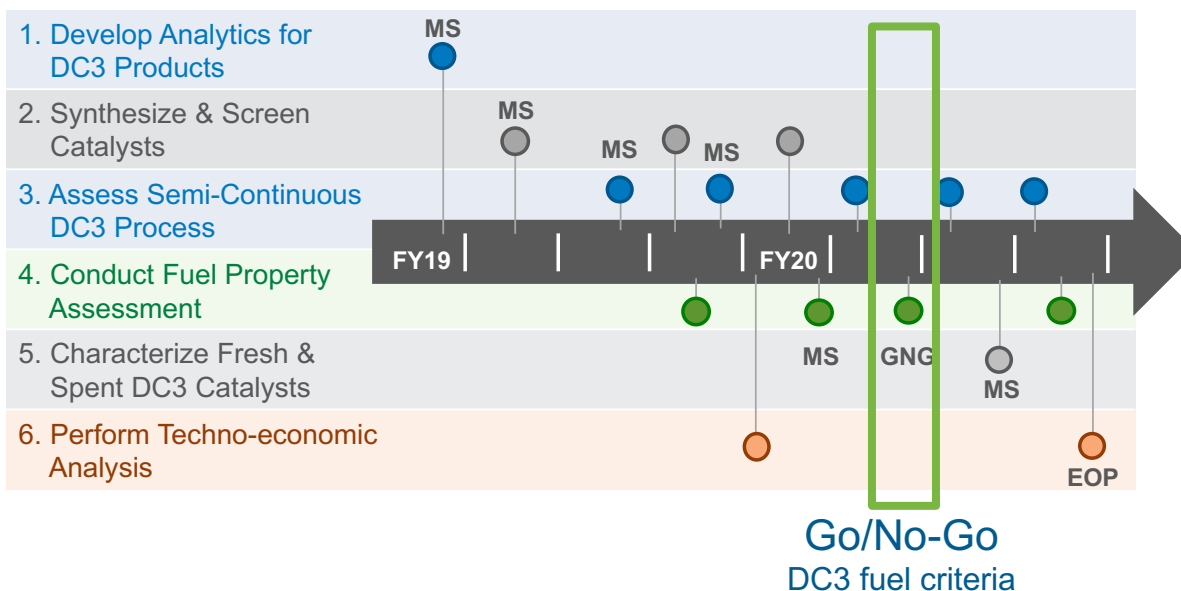
FY20 Deliverables will integrate lessons learned



Biofuel Yield & Quality



FY20 Q2 GNG: Validate $\geq 50\%$ of carbon from delignified hybrid pine can be converted to aliphatic alcohols. Establish that major products are suitable as blendstock at the $\geq 20\%$ level.



Future milestones will address conversion and fuel success criteria

Summary for DC3 Project



Overview

Goal to develop a semi-continuous process for the direct catalytic conversion of cellulosics (DC3) to upgrade delignified biomass and evaluate the resulting oxygenates for light and/or heavy duty fuel.

Approach

- Develop semi-continuous process for residual cellulosics conversion
- Design catalyst to target desirable product composition based on fuel properties
- Leverage ChemCatBio enabling capabilities, Co-Optima fuel properties knowledge, and Lignin First expertise

Technical Progress

- Reproduce current state-of-the art batch DC3 process
- Demonstrate influence of catalyst formulation on liquid product distribution
- Evaluate preliminarily fuel properties of major DC3 alcohol products

Relevance

The DC3 project seeks to upgrade delignified woody biomass to advantaged fuels and provide alternative to enzymatic hydrolysis

Future Work

- Deploy semi-continuous DC3 reactor for with delignified biomass at 5-g scale
- Tailor catalyst and process design for desired fuel targets
- Generate DC3 fuel samples for biofuel validation and inform integrated TEA

**Thank you for listening...
Let's discuss!**



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