

# Catalytic Upgrading of Biochemical Intermediates (CUBI) 2.3.1.101, ...102, ...103, ...104

Jeffrey Linger<sup>1</sup>, Ashutosh Mittal<sup>1</sup>, Jacob Miller<sup>1</sup>,  
Vanessa Dagle<sup>2</sup>, Xiaokun (Claire) Yang<sup>3</sup>, &  
Andrew Sutton<sup>4</sup>

DOE-BETO Peer Review FY23

April 6, 2023





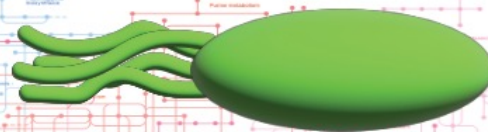
# Approach: Project Overview-Broad Research Strategy



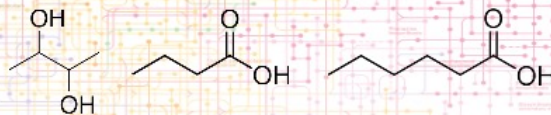
**Biomass**



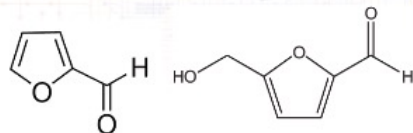
**Sugars**



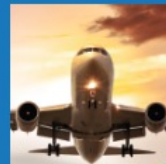
**Biological Upgrading  
to Intermediates**



**Direct Upgrading  
To Intermediates**



**CUBI Directly Synergizes  
with Upstream Projects  
to Upgrade Biochemicals  
To SAF**

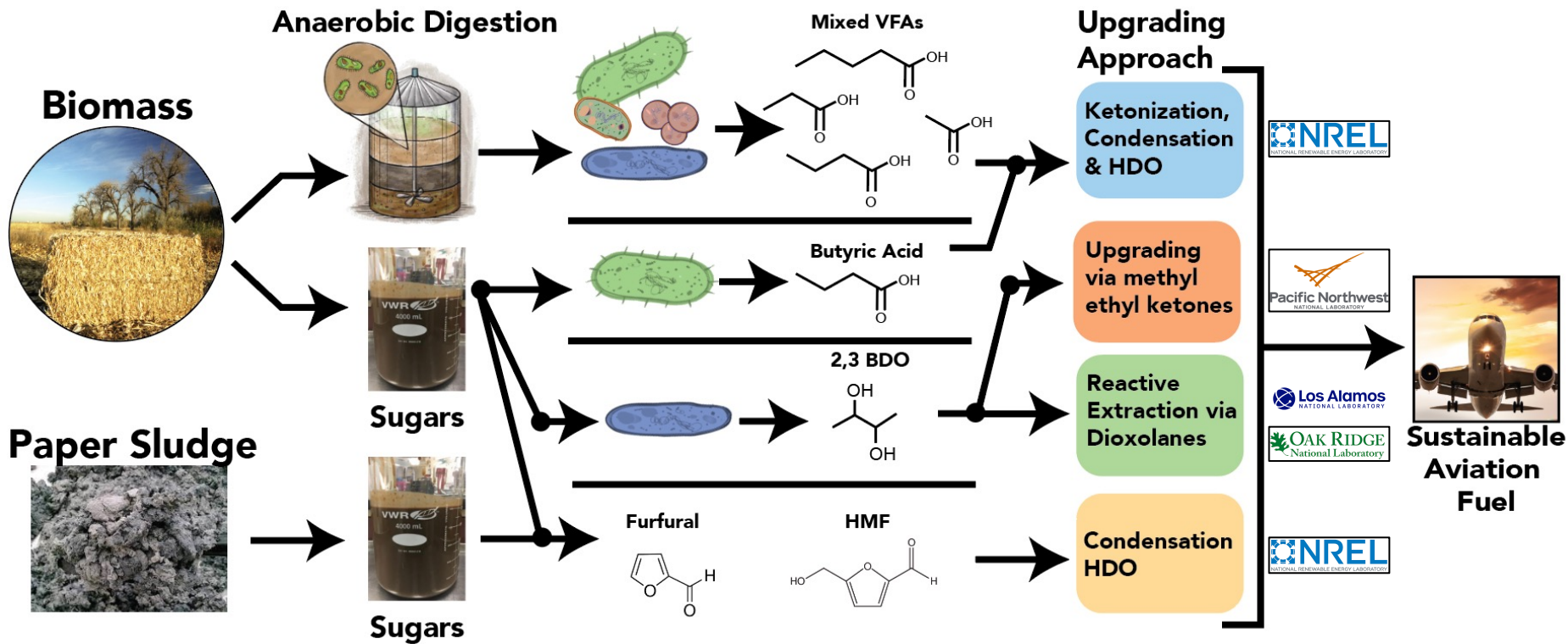


**Sustainable  
Aviation  
Fuel**

**Catalytic Upgrading of  
Biochemical Intermediates**



# Approach: Project Overview- Individual Pathways



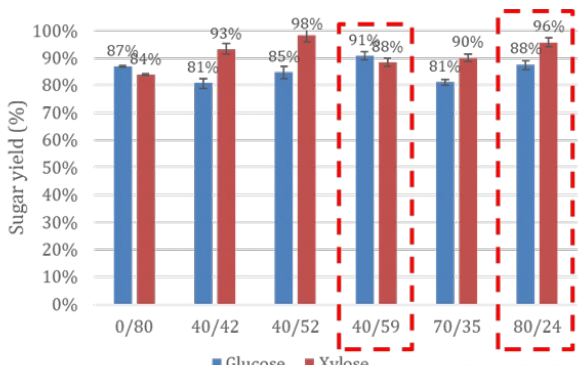
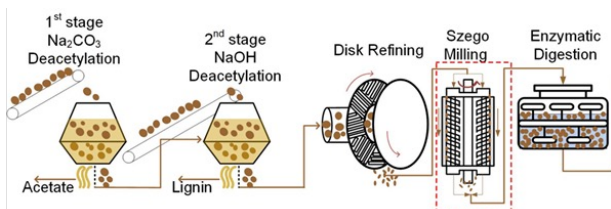
CUBI research is highly integrated with promising upstream processes ...



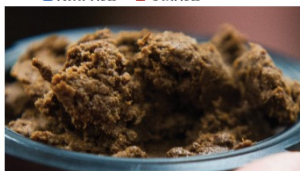


# Approach: Generation of Biochemical Intermediates

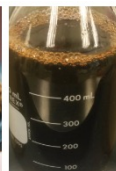
## Biomass To Sugars



Corn Stover

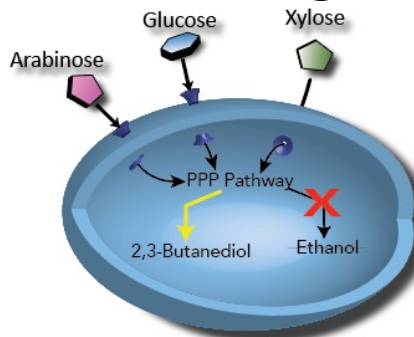


DMR



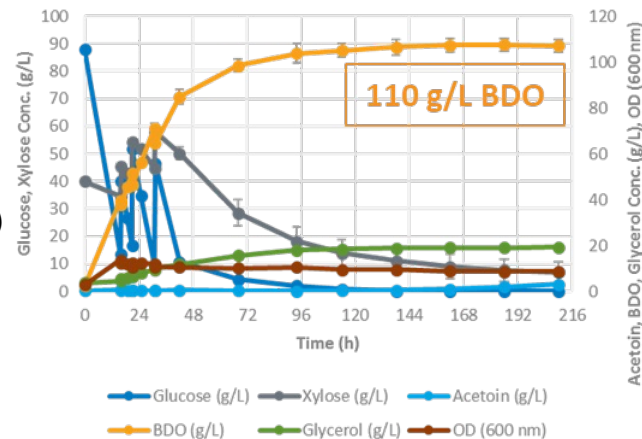
DMR-EH

## Sugars to 2,3-butanediol



**Engineered *Z. mobilis***  
(Targeted Microbial Development)  
Min Zhang

**Fermentation Engineering**  
(Bench Scale Integration)  
Nancy Dowe

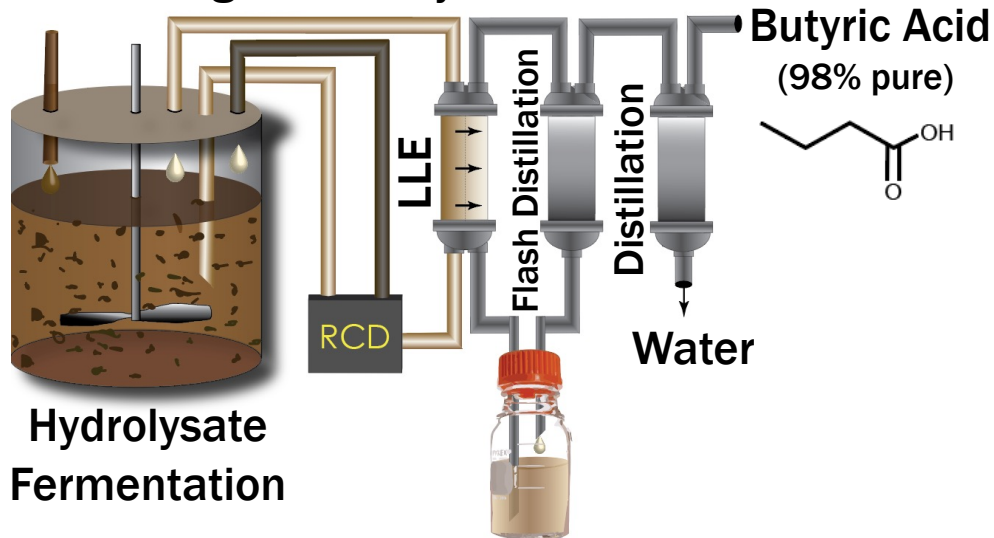




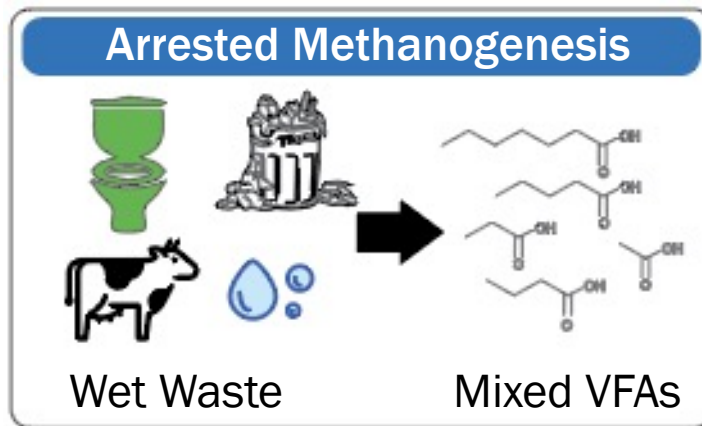


# Approach: Generation of Biochemical Intermediates

## Sugars to Butyric Acid



## Wet Waste to mixed VFAs

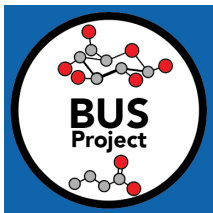


Pilot Scale Reactor System  
for Acids Production from  
Hydrolysate or wet waste



# Approach: Increasing Impact Through Collaborations

Pilot Scale  
Production of  
volatile fatty acids



TEA & LCA  
Analysis



Biochemical Process  
Analysis

Advancing  
carboxylic acid  
separations



Engineering BDO  
Production Strains



TMD



CCPC

CDM

Catalyst  
Deactivation  
Mitigation

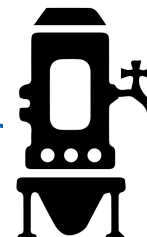
ACSC

Catalyst Design

CUBI

ALDER  
FUELS

VFA Upgrading  
Collaboration



Pilot- Scale  
BDO  
Fermentation

Luxfer-MEL



# Approach: Key Milestones and Go/No Go decision points

FY23

Sep 2023: [Develop butyric acid to SAF blendstock upgrading process](#) in alignment with the acids Biochemical SOT

FY24

Sep 2024 Go/No-Go: **GO-** Demonstrate improvements that validate potential for either or both BDO upgrading pathways to be viable or **No-Go:** PNNL, ORNL, & LANL will work jointly to accelerate the commercial deployment of the preferred pathway to SAF.

FY25

Sep 2025 End of Project: [De-risk end-to-end biochemical intermediate upgrading processes to SAF](#) through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions targeting  $<27 \text{ g CO}_2 \text{ eq/MJ}$  (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.



# Approach: Project Management



**Jeff Linger (PI, NREL)**  
Overall Coordination &  
Biological Integration



**Sonia Hammache  
(TM, BETO)**  
Strategic Guidance

## Interaction Highlights

- Formal monthly team meetings
- Joint milestones and Go/No-Go decisions
- Strategy sessions with upstream technology (feedstocks, biology, fermentation) and TEA/LCA teams.
- Engagement with industrial stakeholders



**Ashutosh Mittal**  
Furan Upgrading



**Jacob Miller**  
Acids Upgrading



**Vanessa Dagle**  
BDO Upgrading  
(MEK)



**Xiaokun (Claire) Yang**



**Andrew Sutton**



**BDO Upgrading (Dioxolane)**

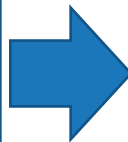
# Presentation Overview: Speakers



Ryan Davis



Progress & Outcomes:  
From a TEA/LCA  
Perspective  
Biochemical  
Platform Analysis  
Project



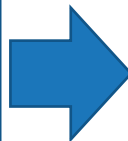
Ashutosh Mittal  
Furan Upgrading



Jacob Miller  
Acids Upgrading



Vanessa Dagle  
BDO Upgrading  
(MEK)



Xiaokun (Claire) Yang  
BDO Upgrading  
(Dioxolane)



Andrew Sutton  
BDO Upgrading  
(Dioxolane)



# Progress & Outcomes: From a TEA and LCA Perspective

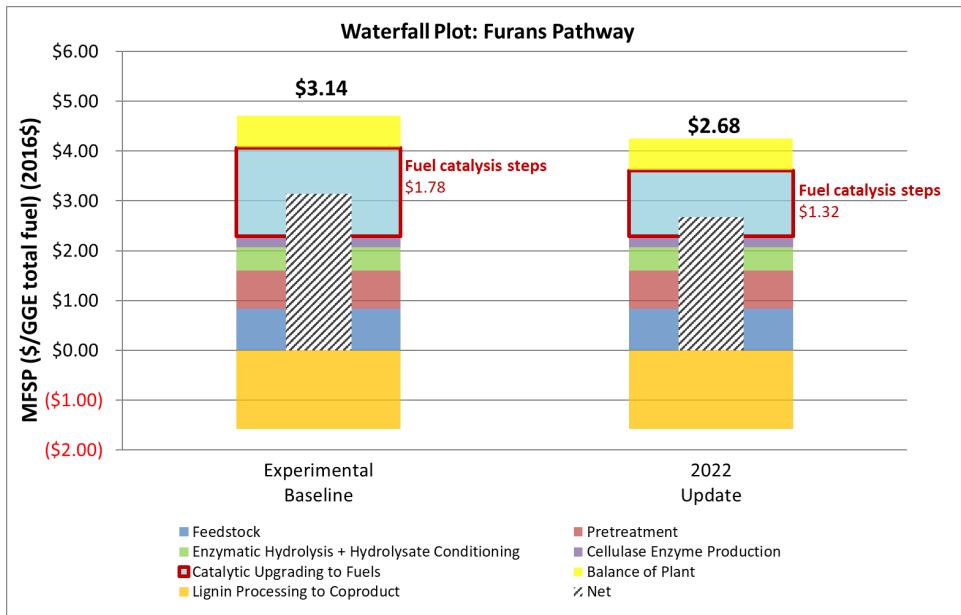
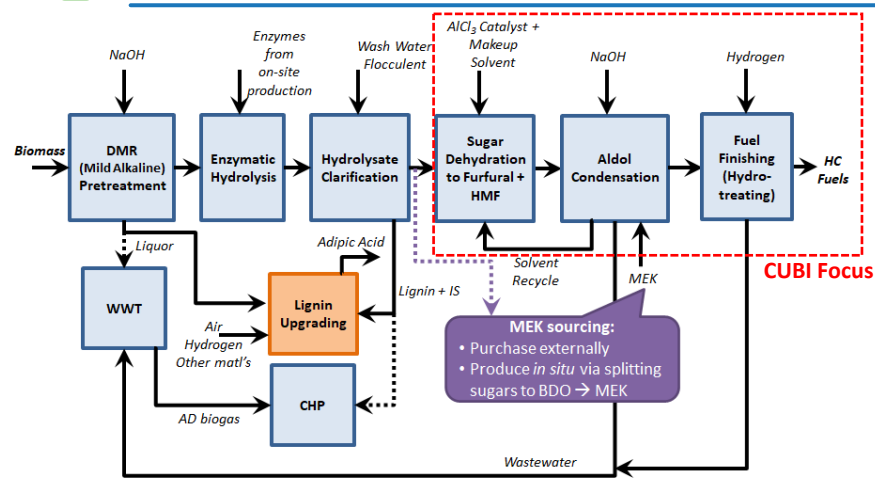
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Ryan Davis, NREL  
Biochemical Platform Analysis





# Furans Pathway: TEA Highlights Improved Process

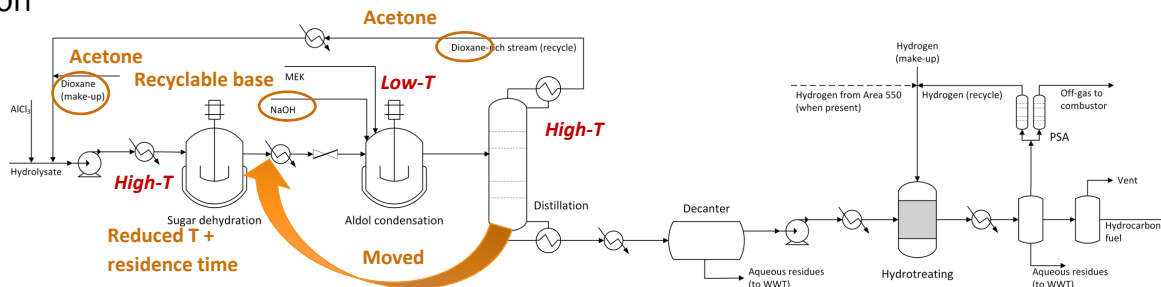


- FY22 Q4: TEA evaluated recent R&D improvements for furans pathway**

- Replaced dioxane solvent with acetone
- Moved solvent recovery before condensation
- Lower T + residence time for dehydration
- Recyclable base for aldol condensation

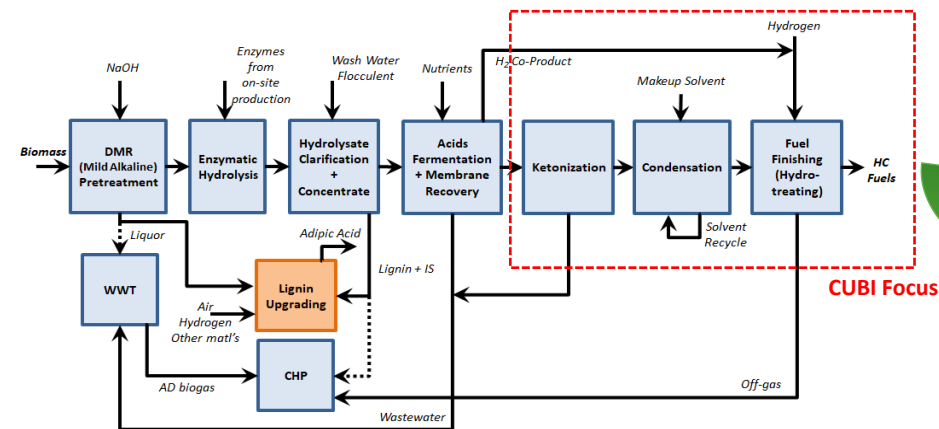
- Reduced baseline MFSP by \$0.46/GGE (exceeded 25% catalysis target)**

- FY22 now meets/exceeds 2030 target for furans catalysis portion

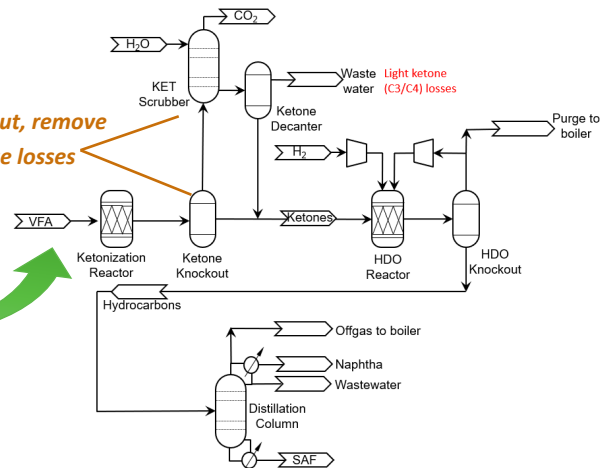




# Acids Pathway: Optimization for Wet Waste VFA

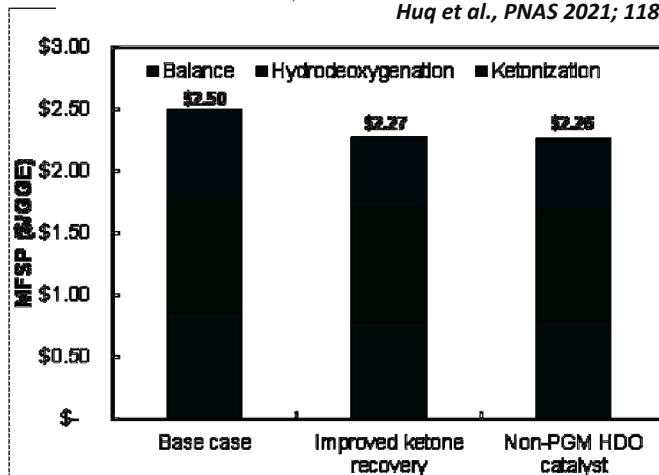


Chilled ketone knockout, remove scrubber = minimize losses



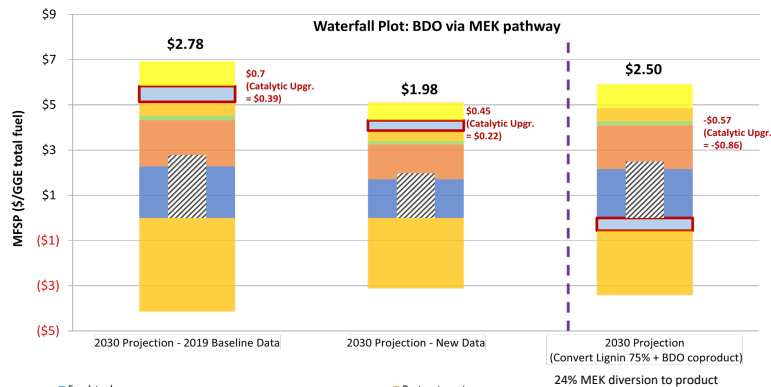
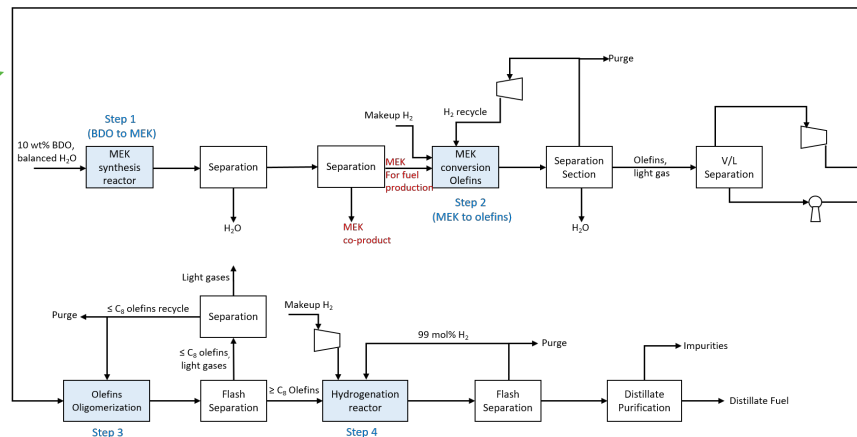
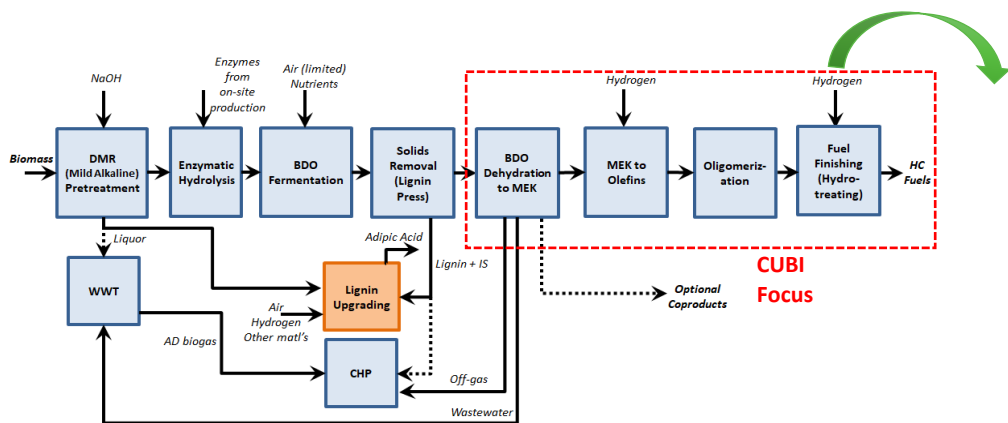
Huq et al., PNAS 2021; 118(13)

- Biochem acids catalysis steps all nearly at/exceeding 2030 goals
  - Exception: ketonization WHSV updated in 2022 to  $0.4 \text{ h}^{-1}$  (vs prior baseline of  $4.0 \text{ h}^{-1}$ ) based on new catalyst deactivation findings
- More recent CUBI work has shifted focus to wet waste VFA pathway – more optimal catalytic route to SAF:
  - Eliminates condensation step
  - Produces fuel product more directly in SAF boiling range
- FY22 CUBI analysis identified further VFA-SAF cost reduction opportunities, via:
  - Improved recovery of volatilized ketones from  $\text{CO}_2$  vent =  $\$0.23/\text{GGE}$
  - Replacing  $\text{Pt}/\text{Al}_2\text{O}_3$  with  $\text{NiMo}/\text{Al}_2\text{O}_3$  catalyst for ketone HDO =  $\$0.01/\text{GGE}$





# BDO/MEK Pathway: TEA Highlights Improved Process

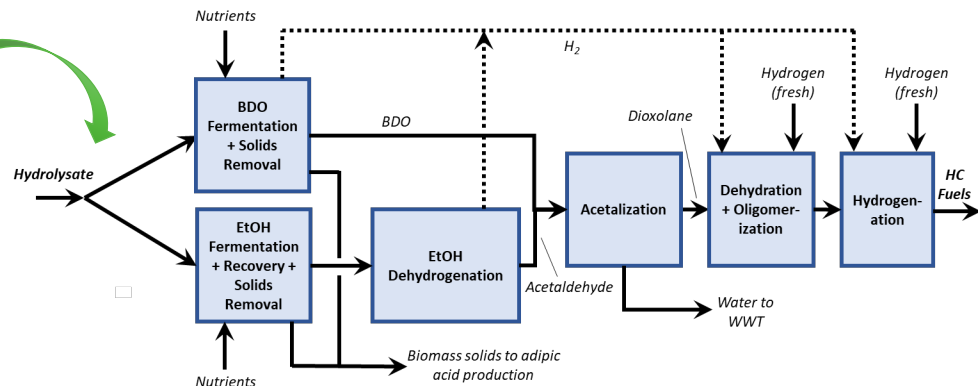
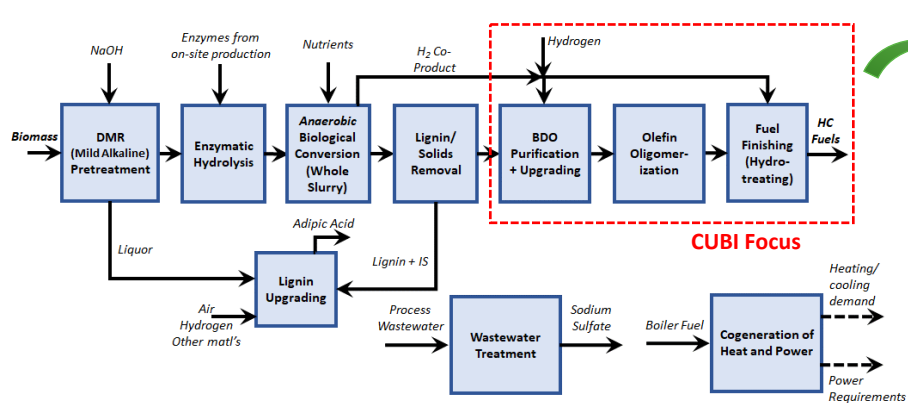


- Developed 2-step approach to convert BDO to olefins (SAF precursor) via MEK intermediate without energy-intensive separation of BDO from water
- New TEA improvements reduced baseline MFSP:
  - Improvements in C efficiency
  - Facile separation of MEK from water after step 1 = smaller reactor, no need for water vaporization in step 2
  - Improved operating conditions (throughput, temperature, pressure)
- FY22 now meets/exceeds 2030 target for BDO catalysis portion
- **Updated 2030 case reflects highly favorable MFSP potential <math>< \\$2/\text{GGE}</math>**
- TEA + LCA identified opportunities for further improvement to reduce GHG emissions: operate step 1 in liquid phase

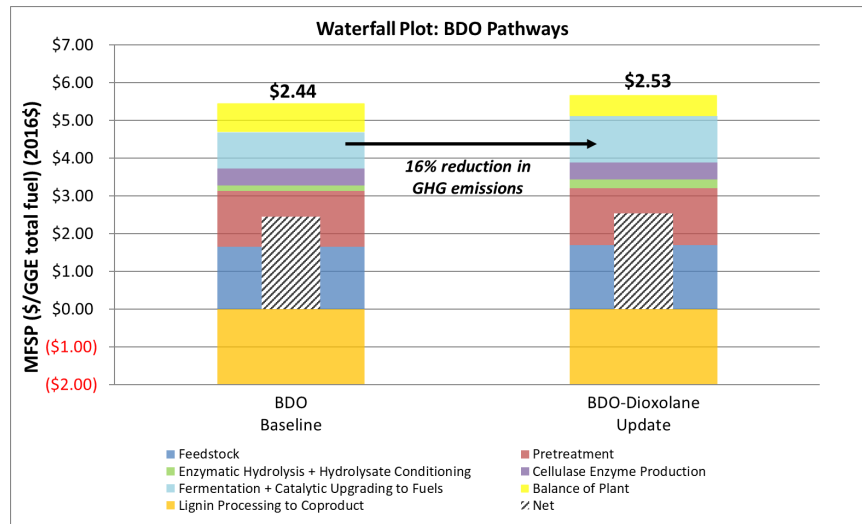




# BDO/Butene Pathway: TEA for Novel BDO Recovery



- BDO pathway holds promise for either fuel or chemical production, but challenged by high energy use for aqueous BDO upgrading (90%+ water, 250 °C)
- New work under CUBI and SepCon investigating novel approach to isolate BDO via dioxolane intermediate
  - Dioxolane phase separation + direct upgrading to butene
  - Reactive extraction: reverse to aldehyde (recycle) + BDO
- FY22 Q2 TEA found **comparable MFSP (<5% increase) + 16% lower GHG potential**
  - Similar or better results seen under SepCon for reactive extraction
- Could be a game-changer for the BDO pathway, and will be further investigated under NREL BC Analysis task in FY23



# Catalytic Upgrading of Mixed Sugars Derived Furfurals to SAF

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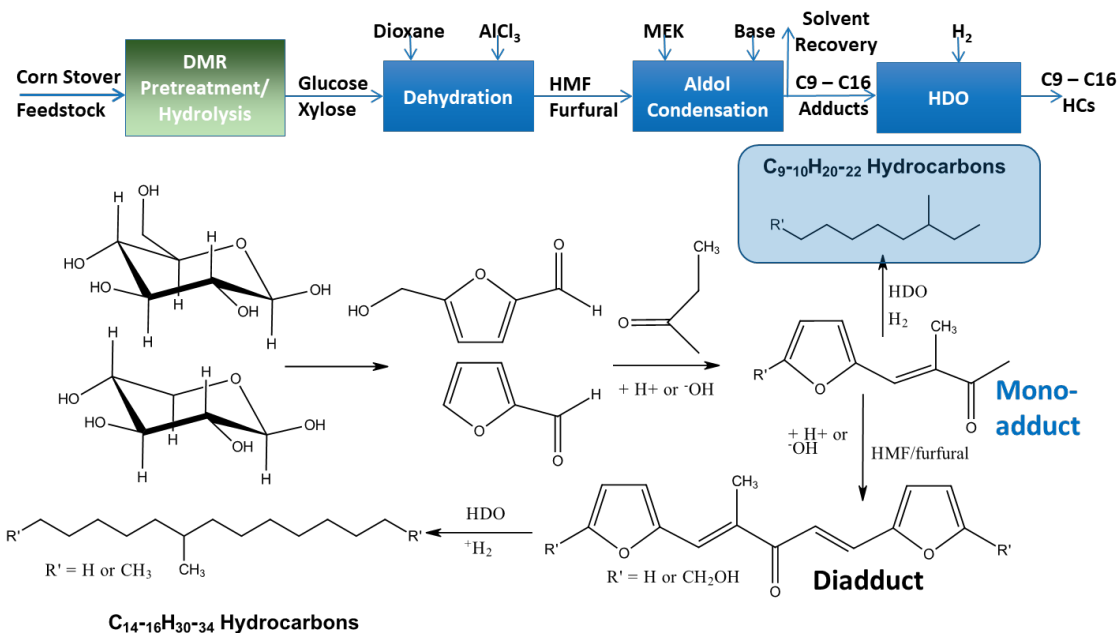
Ashutosh Mittal, NREL





# Furfural Upgrading to SAF : Project Overview

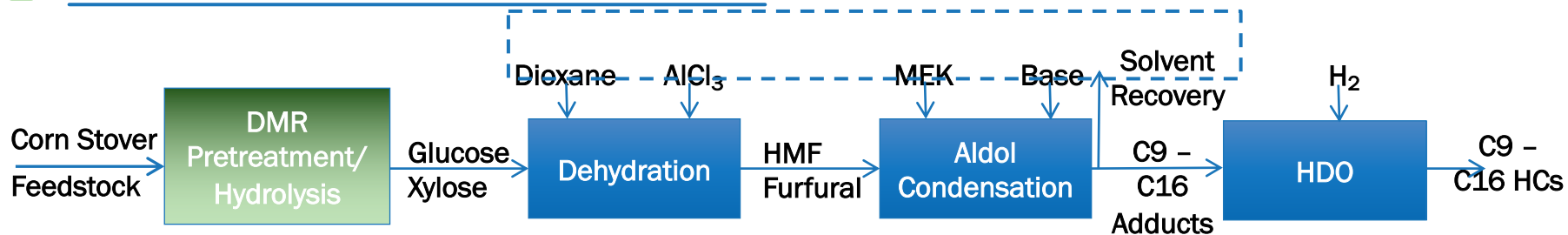
## Overview of the Furfurals Upgrading Pathway



- R&D is focused on the 3 conversion processes shown in the 3 blue boxes
- Dehydration of sugars to furfurals using catalysts that are a mixture of Lewis and Bronsted acids in an organic/aqueous solvent
- Aldol condensation of furfural mixture with bio-MEK to produce C9-C16 intermediates
- Hydrodeoxygenation of intermediates to hydrocarbons using metal catalysts on silica-alumina supports
- A change in the aldol condensation to favor monoadduct intermediates would shift the final hydrocarbons more into the jet fuel distillation



# Furfural Upgrading to SAF : Project Overview/ Approach



- Prior to 2021:

- Used azeotropic solvent (dioxane) in dehydration reaction
- Used homogenous catalyst (NaOH) in aldol condensation reaction; C9 - C16 target intermediates

- Since 2021:

- FY22-Q2: Characterize opportunities for LCA improvements for CUBI catalytic upgrading pathways.
- FY22-Q4: Reduce the MFSP contribution of the catalytic upgrading process section by 25% as compared to the 2020 TEA design case.
- Approach: To achieve TEA/LCA metrics, alternative approaches were considered beyond the base-case process configurations by employing several catalytic process improvement strategies, including:
  1. Replacing dioxane with a non-azeotropic solvent, such as, acetone
  2. Identifying alternatives to NaOH that are more easily recycled and contribute less to CO<sub>2</sub> emissions
  3. Improved aldol condensation of ketones with biomass hydrolysate derived furfurals targeting C9-C10 intermediates which after hydrodeoxygenation are suitable for SAF

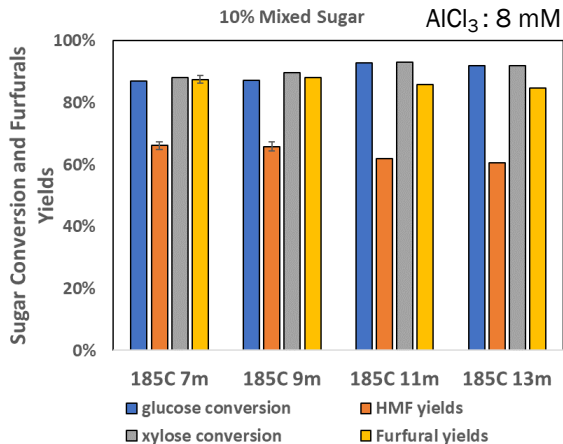


# Progress & outcomes: Dehydration of Sugars to Furfurals Using Acetone

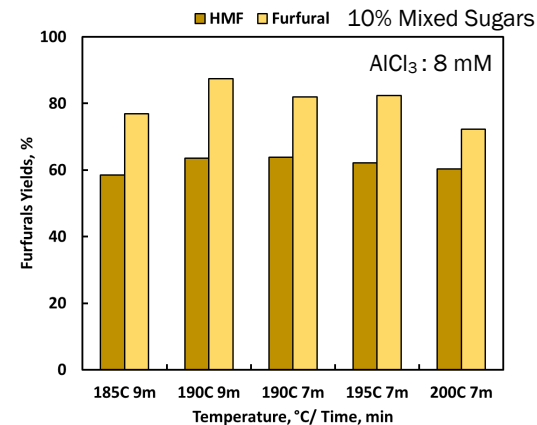
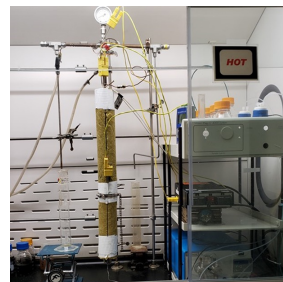
## Objectives:

- Identify optimum reaction conditions in batch reactions to replace dioxane with non-azeotrope solvent (acetone)
- Optimize reaction conditions for scaling-up dehydration of sugars to furfurals in a tubular flow reactor

## Furfurals Production in Microwave Reactor



## Furfurals Production in Flow Reactor



## Key Outcomes:

- Dioxane replaced with non-azeotropic solvent (acetone), optimum reaction conditions obtained in batch reactions (185 °C, 7 min)
- Dehydration of sugars to furfurals scaled-up in a tubular flow reactor (1 L/ day)



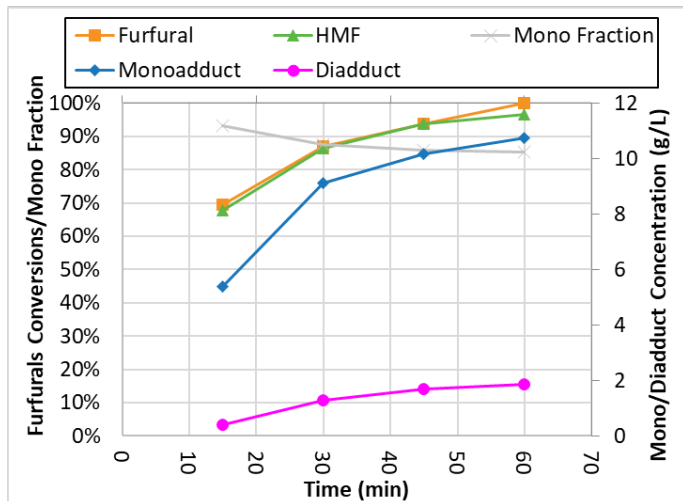


# Progress & outcomes: Aldol Condensation to Monoadduct with Solid Base Catalysts

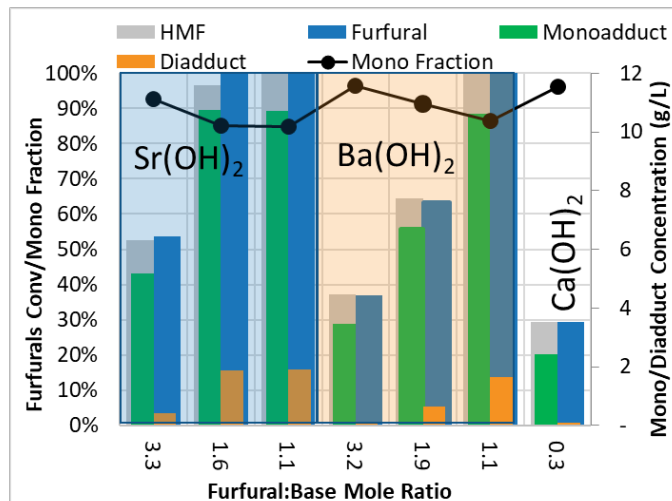
## Objectives:

- Improved aldol condensation of ketones with biomass hydrolysate derived furfurals targeting (C9 - C10) intermediates which after hydrodeoxygenation are suitable for SAF
- Identifying alternatives to NaOH that are more easily recycled and contribute less to CO<sub>2</sub> emissions

### Furfurals:Sr(OH)<sub>2</sub> mole ratio 1.6



### Comparison of different solid bases for aldol condensation



## Key Outcomes:

- Best results of aldol condensation to monoadduct were obtained with Sr(OH)<sub>2</sub>
- Solid bases did not dissolve in reaction solvent;
- The LCA found the potential to reduce GHG emissions by roughly 4%



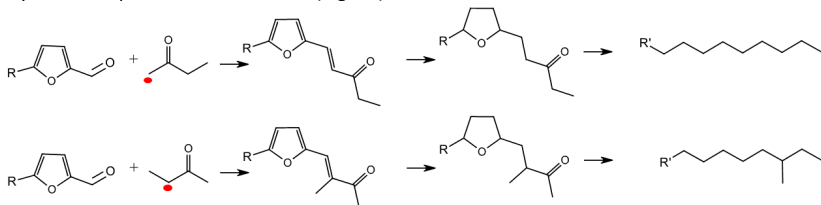
# Progress & outcomes: Hydrodeoxygenation of Aldol Condensates

## Objectives:

- Develop better understanding of catalyst roles in HDO of aldol condensation intermediates
- Investigate the effects of substrate concentration, varied catalyst loading, and Pd or Pt Catalyst on MS-13 Support

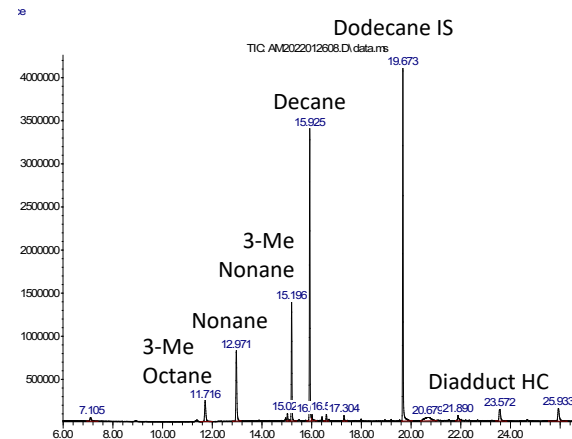
Catalyst	Pd/MS-13	Pd/MS-13	Pt/MS-13	Pt/MS-13	Pt/MS-13	Pd/MS-13
Substrate/ Catalyst weight ratio	7.8	3.9	3.9	2.6	2.0	2.0
Aldol condensates concn. (g/mL)	0.40	0.20	0.20	0.20	0.10	0.10
C8-C10 HC	59.68	55.56	57.11	58.25	34.30	35.89
C13-C16 HC	5.93	6.22	4.96	4.97	3.08	3.86
Cycloparaffins	3.65	1.95	3.35	2.68	0.62	0.56
Oxygenates	25.99	nd	nd	nd	nd	nd
Isolated yield (Wt%)	56.7%	51.6%	48.2%	52.3%	50.2%	51.1%

Hydrocarbon product concentrations (mg/mL); nd = not detected



- Predominance of n-alkanes is because of higher acidity of methyl protons
- Attack at methyl C favored over methylene C

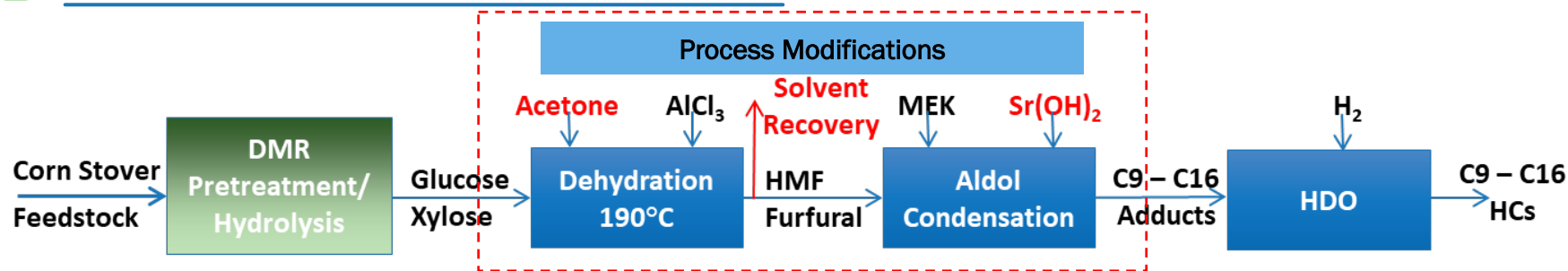
## GCMS Hydrocarbon product



## Key Outcomes:

- HDO of intermediates gives n-, iso- and cyclic alkanes
- Small amounts of cycloparaffin products, e.g., butyl cyclohexane, pentyl cyclopentane
- GCMS and NMR results indicated only very low levels of oxygenated products in some samples

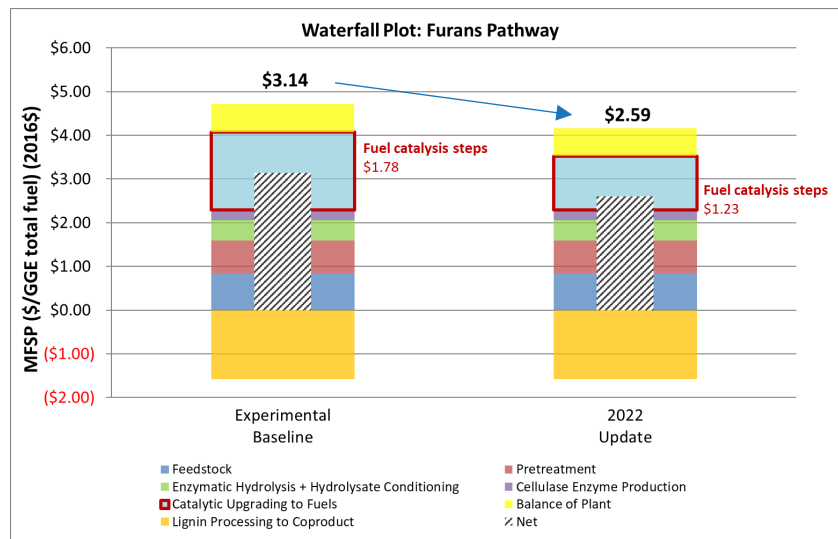
# Progress & outcomes: TEA/ LCA



## Following operational modifications were implemented

- Solvent used in the sugar dehydration reaction: dioxane replaced with **acetone**
  - Solvent recovery point: modified to **before** the aldol condensation step rather than **after**
  - Temperature of the sugar dehydration reaction: **190°C** instead of **230°C**
  - Reaction time: **5 - 7 min** instead of **15 min**
- Aldol condensation catalyst: recoverable alkali – **Sr(OH)<sub>2</sub>** – instead of **NaOH**
- **Catalysis-attributed contributions to MFSP are shown to be reduced from \$1.78/GGE to \$1.23/GGE, a 31% reduction > 25% reduction target**

## Technoeconomic Analysis

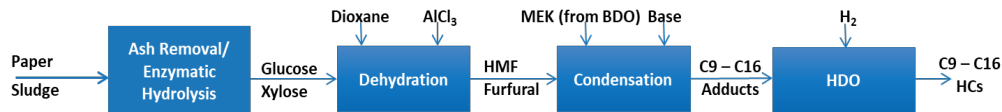




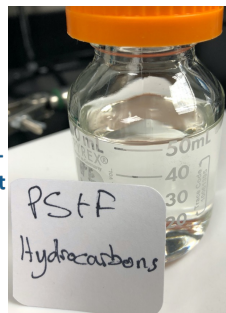
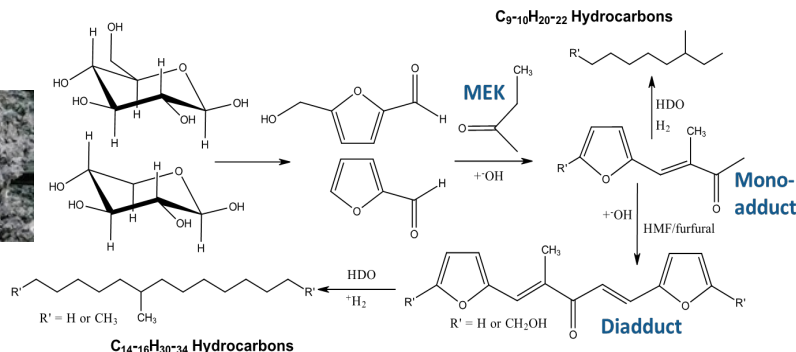
# Impact: Furfural Upgrading to SAF Adapted to Paper Sludge Waste

## BETO FOA with NC State for Upgrading Carbohydrates in Paper Sludge Waste to Hydrocarbons

- Evaluate if the process for converting carbohydrates in biomass could be adapted to paper sludge waste



Paper Sludge



## Fuel Properties of Hydrocarbon Product

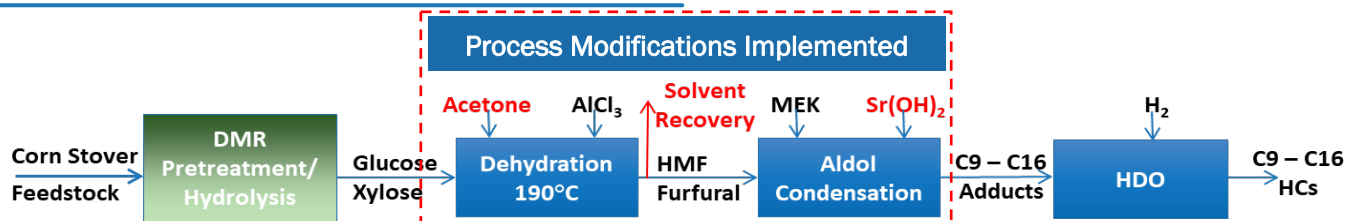
CH content (wt%)	84.95%C 14.10%H
O content (wt%)	0.059 ± 0.004
n-alkanes	53.7 wt%
iso-alkanes	39.7 wt%
cyclo-alkanes	6.6 wt%
Freezing point (°C)	-48.1
Cetane number	65.0
HHV (MJ/kg)	46.7
Density at 15°C (g/cm <sup>3</sup> )	0.792
Energy density (MJ/L)	37.0

## Outcomes:

- 50 mL of hydrocarbon product made for fuel property testing. Scaling-up to produce 1 liter hydrocarbon product.
- Fuel properties indicate it could be excellent for blending into jet or diesel fuels.
- Simulated distillation indicated 61% in jet fuel boiling range, 67% in diesel fuel range



# Summary of key accomplishments, outcomes and impact since 2021



## Technical progress & Outcomes since 2021

- Implemented the following process improvement modifications in dehydration and aldol condensation steps:
- **Dehydration:** (1) In the sugar dehydration reaction azeotropic solvent (dioxane) replaced with non-azeotropic solvent (acetone)
- (2) Solvent recovery point modified to before the aldol condensation step rather than after resulting in energy savings
- (3) Low reaction severity: (a) Optimized the sugar dehydration reaction temperature from 230°C to 190°C, and (b) Reaction time from 15 min to 7 min resulting in energy savings
- **Aldol condensation:** (1) Homogeneous base catalyst (NaOH) replaced with a recoverable alkali (Sr(OH)<sub>2</sub>)
- (2) Improved aldol condensation targeting (C9 - C10) intermediates
- **TEA/LCA:** Catalysis-attributed contributions to MFSP are shown to be reduced from \$1.78/GGE to \$1.23/GGE, a 31% reduction > 25% reduction target

## Impact since 2021

- De-risk technology for catalytic conversion of renewable biomass- and waste-derived sugars and sugar-derived intermediates into sustainable aviation fuels (SAF)
- Demonstrated furfural upgrading to SAF on biomass-derived sugars and adapted and implemented to paper sludge waste
- **Environmental: Decarbonization through GHG emission reduction**
- Demonstrated a viable technology for replacing fossil-derived jet fuel with renewable biomass-derived SAF
- **Publications/ intellectual property**
- Published a “mini-design report” for this pathway (2021)
- US Patent App. 17/666,493, 2022 – Simultaneous dehydration of glucose and xylose to furfurals using heterogenous solid acid catalysts: A Mittal, DK Johnson

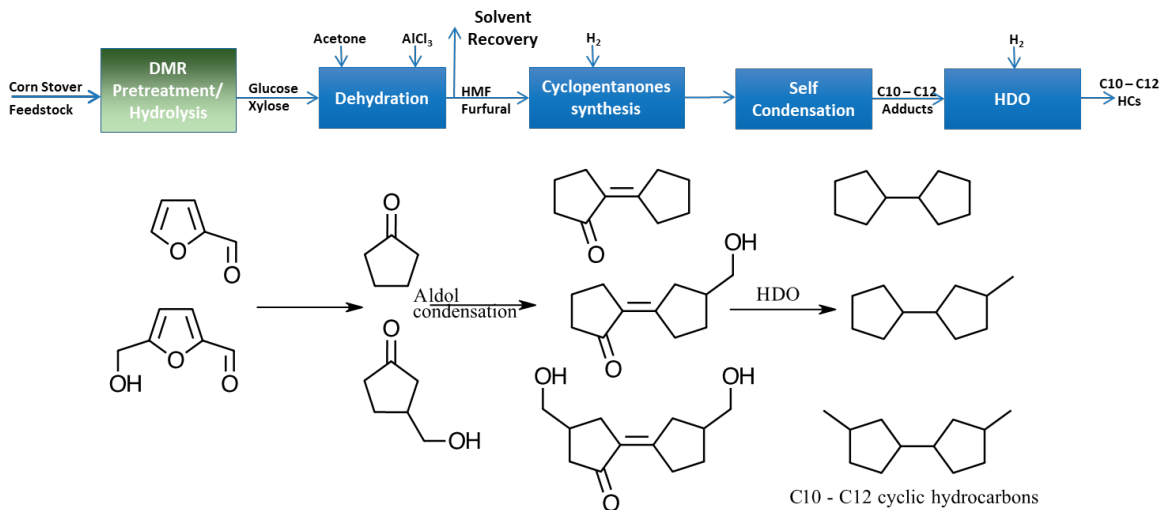




# Future Work

## Transitioning from Linear to Cyclic Paraffins

- Overall concept to convert mixed sugars to jet fuel range hydrocarbons by upgrading furfurals via conversion to cyclopentanones followed by aldol condensation of the cyclopentanones and then HDO



**FY2024 Go/No-Go:** In the critical step of furfurals-to-cyclopentanones, achieve a 50% carbon-yield using a biomass hydrolysate-derived furfural mixture.

### Expected Outcomes to improve TEA/LCA:

- Dehydration – Acetone, non-azeotropic organic solvent, solvent recovery after dehydration
- Self-condensation – Furfurals derived cyclopentanones, no imported ketone needed
- HDO severity – Moderate, 250°C no ring opening needed
- Lower GHG emissions – Less  $H_2$ , less energy for solvent recycle, lower T HDO
- HC product – mostly  $C_{10}$ - $C_{12}$  cycloalkanes
- Energy density of HC product – ~40 MJ/L
- Fuel props. – BPt 190-234°C, FPt -35°C  
FlashPt ~40°C, visc @-20°C 2.6 mm<sup>2</sup> s<sup>-1</sup>

# Volatile Fatty Acids to SAF

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Jacob Miller, NREL



# CUBI Acids

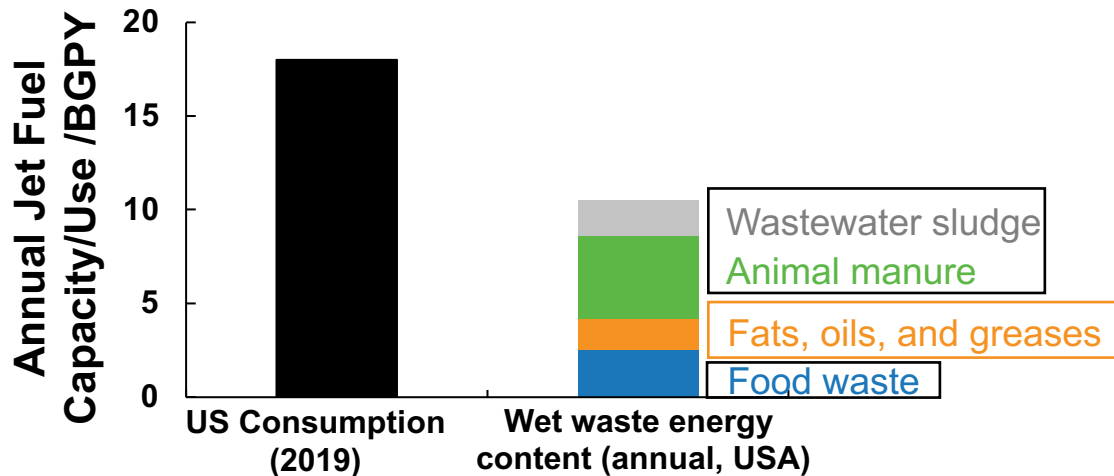
## Upgrading: Project Overview/Approach

- Feedstock: (i) Wet waste or (ii) waste sugars
- Biological upgrading, separations → Carboxylic acids
- Heterogeneous catalytic reactions in flow reactors: Ketonization, hydrodeoxygenation (HDO), cyclization
- Target product: Sustainable aviation fuel (SAF)





# Approach: Wet waste valorization state of technology



- **FOG to SAF:** Already industrially practiced
- **All other wet wastes:** No commercialized SAF pathways (84% of total volume!)

Leading commercialized wet waste valorization technology: Anaerobic digestion to biogas → combined heat/power or bio-methane.

- Renewable electricity value: **\$13.01/MMBtu**
- Renewable methane value: **\$19.00/MMBtu**
- SAF value: **\$57.04/MMBtu**

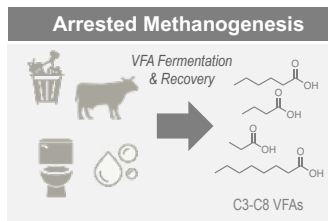
Skaggs et al. *Renewable and Sustainable Energy Reviews* (2018) 82, 2640-2651.  
U.S. Bureau of Transportation Statistics (2022).

*Value of wet waste **maximized** when upgraded to SAF!*



# Approach and progress update: Carboxylic acids to SAF

*Biochemical process → Thermochemical catalysis (commercial catalysts) → SAF*



- Carbon efficiency (acids → HCs): 75-90%
- Blendable up to 70% in Jet A
- -55 gCO<sub>2</sub>eq/MJ

## Prior to 2021

- Demonstrated all steps
- Identified preferred catalysts & operating conditions
  - Condensation step demonstrated only in batch mode
- Demonstrated conversion of biogenically-derived carboxylic acids to SAF blendstock, TEA, LCA, fuel property measurement

## Since 2021

- In-depth, scale-up-oriented study of ketonization step
  - Kinetics and industrial-scale reactor design
  - Developed understanding of catalyst deactivation
- Developed a flow reactor process for light ketone upgrading to replace condensation step



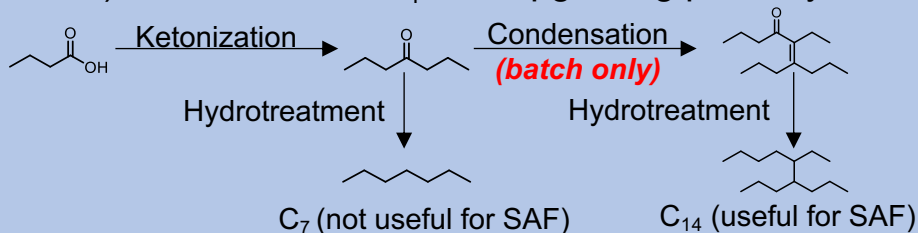


# Approach: Go/No-Go

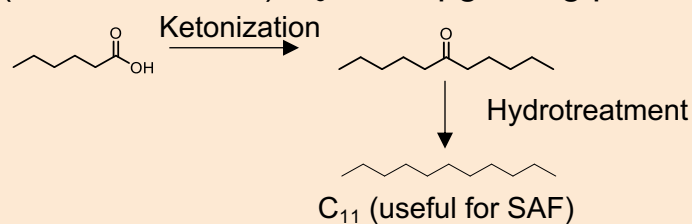
- **Go/No-Go (FY24 Q4):**

- Convert biogenically-sourced **butyric acid** to 100 mL sustainable aviation fuel blendstock
- Target **overall process carbon yield of 60%**.
- Harmonize findings to align SOT-relevant research targets

(Former) state-of-the-art  $C_4$  acid upgrading pathway:



(Current, former)  $C_6$  acid upgrading pathway:



**$C_6$  acids more readily converted to SAF than  $C_4$  acids— $C_4$  acids upgrading process needed**



# Approach: DEI, Cross-cutting collaborations

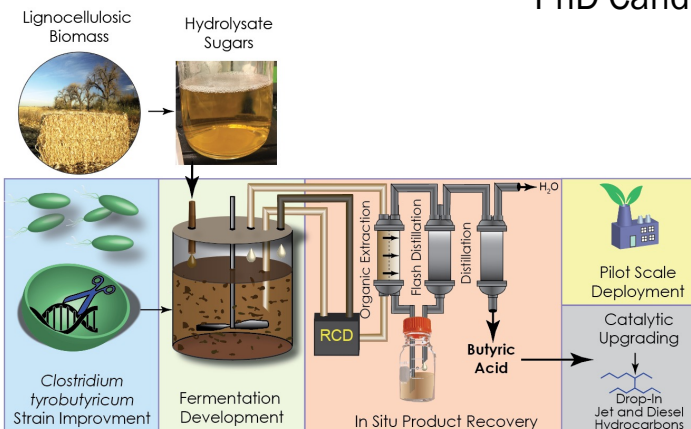
- Training young researchers
- Collaborations within BETO-funded work
  - Steering BETO Biological Upgrading of Sugars (BUS) to focus on production of *hexanoic* ( $C_6$ ) instead of *butyric* ( $C_4$ ) acid production to optimize SAF applicability
  - CCPC: Ketonization density functional theory modeling, kinetics (Rajeev Assary, Hieu Anh Doan—Argonne National Laboratory)



Maya Al Abri- NREL Intern



Raiven Balderas-CO  
School of Mines Chemistry  
PhD Candidate



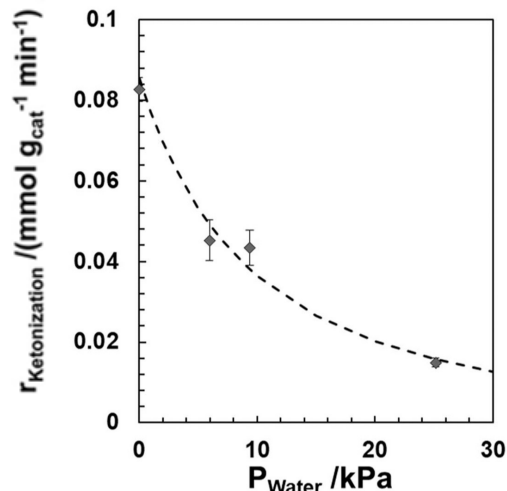
**Important DEI role and collaborations**



# Progress & Outcomes: Ketonization reactor

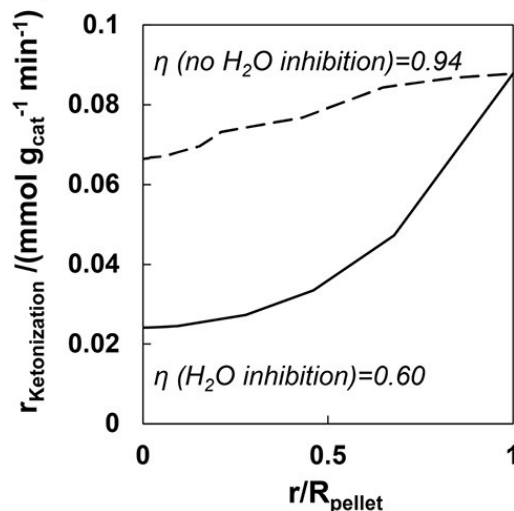
Goal: Derisk implementation of ketonization in an industrial-scale reactor.

1) **Kinetics** over commercial **catalyst powder**: Water (co-product) inhibits rates

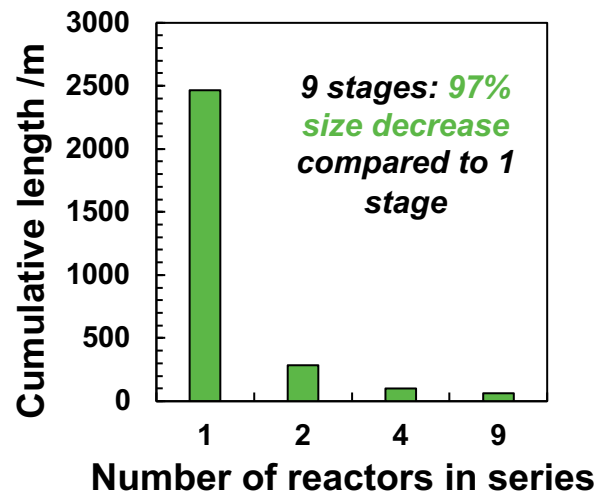


Conditions:  $T = 350 \text{ }^\circ\text{C}$ ,  $P_{\text{C}_6 \text{ acid}} = 0.8\text{--}75 \text{ kPa}$ ,  $P_{\text{Water}} = 0\text{--}25 \text{ kPa}$ ,  $m_{\text{ZrO}_2} = 0.05\text{--}1 \text{ g}$ .  $X_{\text{Hexanoic acid}}$  is usually  $<10\%$ . Error bars: Standard deviations of rates

2) Kinetic **parameter estimation, modeling**: Predict transport limitations over commercial **catalyst extrudates**



3) **Industrial-scale reactor model**: Multi-stage reactor with interstage water separation enables smaller reactor size



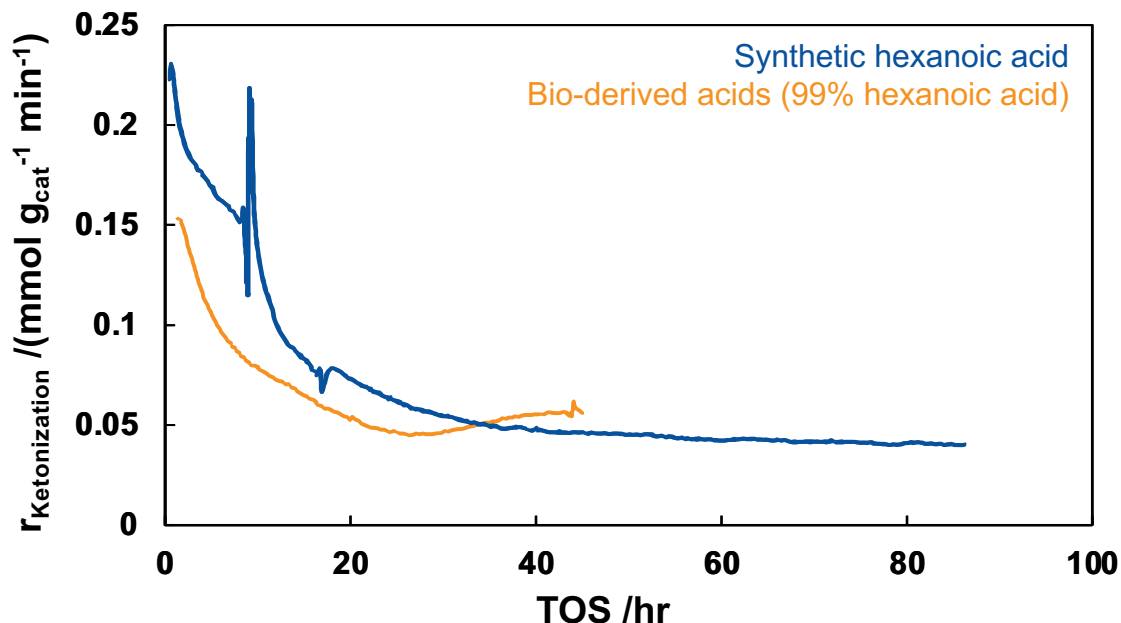
**Key finding: Water inhibition of ketonization rates can be mitigated by water removal.**



# Progress & Outcomes: Ketonization deactivation

Goal: Derisk deactivation of  $ZrO_2$  catalyst during ketonization

Partial conversion ketonization over commercial  $ZrO_2$  powder:



- Ketonization rates **drop 5-6x** during first ~50 hours on stream
- Ketonization rates **stabilize past this point**—*design process around these stable rates to run for 1000s hours on stream*
- Biogenic impurities—**no noticeable further deactivation**
- Adjusting reactor size for deactivation only increases MFSP by \$0.04/gal

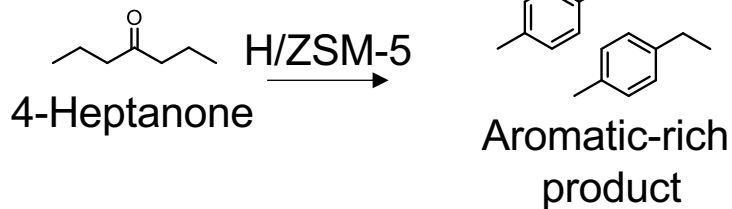
Conditions:  $T=380^{\circ}\text{C}$ , Commercial  $ZrO_2$  powder,  $P_{\text{Tot}}=1.5$  bar (biogenic) or 0.89-0.96 bar (neat  $C_6$ ), He sweep gas,  $\text{WHSV}=11 \text{ hr}^{-1}$

**Key finding: Catalyst deactivation necessitates slightly higher capital costs but is manageable.**



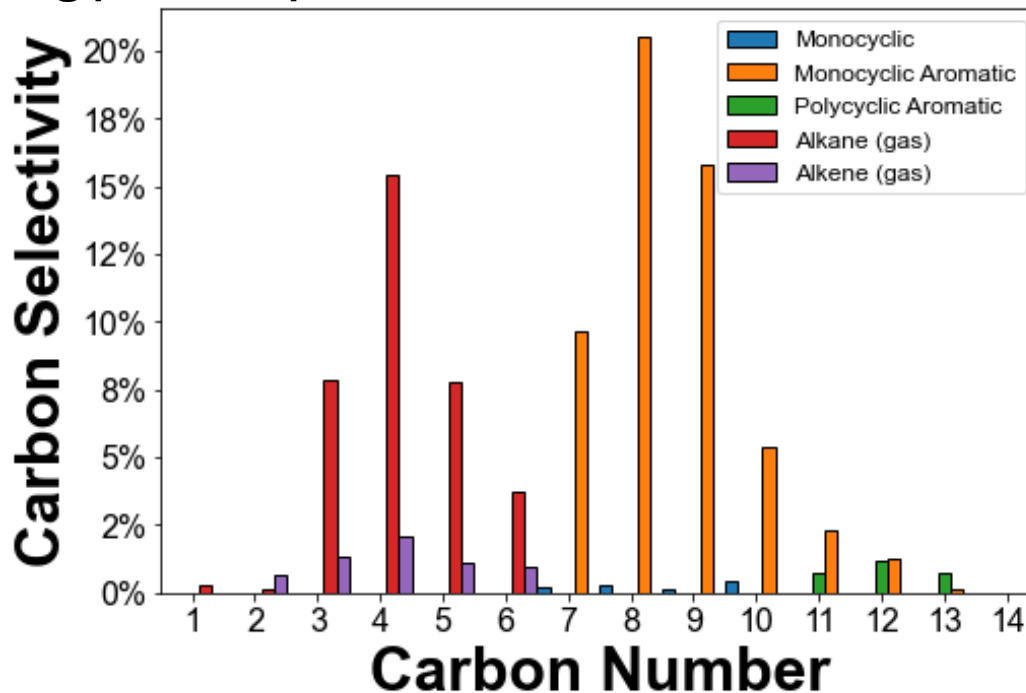
# Progress & Outcomes: Value from light acids

Goal: Find light acid or ketone upgrading process operable in a flow reactor



**C<sub>3-7</sub> ketone upgrading over H/ZSM-5:**

- Flow process
- Oxygen-free product without H<sub>2</sub> addition
- Aromatics useful as SAF or fine chemical precursors



Conditions: T=350°C, P=137 kPa, P<sub>4-Heptanone</sub>=13 kPa, Balance He. He flowrate: 30 sccm. m<sub>H/ZSM-5</sub>=1 g, WHSV=0.95 hr<sup>-1</sup>, 19-25 hours on stream

**Key finding: Light ketone cyclization over H/ZSM-5 enables utilization of light acids in continuous reactor**





# Impact: Alder Fuels partnership

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**1) ~1 gallon/day ketonization demonstration at NREL (2023)**



**DOE VFA-SAF Scaleup of Bench Applications (SCUBA), Alder Fuels (Prime)**

**2) Intellectual property to be licensed by Alder Fuels**

**A L D E R**  
**F U E L S**





# Summary of key accomplishments, outcomes, and impact since 2021

## Technical progress & Outcomes since 2021

### ➤ Achieved all milestones

- Demonstrated process improvements leading to 10% MFP reduction
- TEA/LCA findings contributed to updated Biochemical State of Technology reports

### ➤ Advanced understanding of key parameters governing ketonization reactor design

- Identified inhibition of rates by water as a key factor influencing necessary reactor size and formulated separations strategy to mitigate this
- Determined that catalyst deactivation (via carbon laydown or impurity poisoning) does not eliminate all reactivity

### ➤ Developed new light ketone upgrading process

- New light ketone upgrading process is operable in flow reactors, forms an aromatic-rich SAF-range product at ~50% selectivity

### ➤ Initiated LCA that identified natural gas and electricity as the main contributors to GHG, helps understand how to reduce GHG emissions

## Impact since 2021

### ➤ Results dissemination

- One publication each in FY21 and FY22: 10.1021/acs.iecr.1c04548, 10.1073/pnas.2023008118
- Presentations at ACS (FY21), AIChE (FY22), and NAM (FY22) conferences

### ➤ Commercialization progress

- One US patent in process, to be licensed by Alder Fuels (US20210188734A1)
- Scaleup of Bench Applications (SCUBA) FOA work to start in FY23

### ➤ Stakeholder engagement

- Attend bi-weekly ChemCatBio (CCB) meetings, annual all-hands (CCB) meetings & monthly CUBI meeting
- Close collaboration with Alder Fuels carboxylic acids to SAF upgrading efforts

### ➤ Close collaboration with other BETO projects to refine strategy

- Helped Biological Upgrading of Sugars project expand focus to make C<sub>6</sub> acid product
- Key contributions to commercialization understanding from CCPC

# Catalytic Upgrading of 2,3-butenediol to SAF Via Methyl Ethyl Ketone (MEK)

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Vanessa Dagle, PNNL



# Task Overview

## Objective

- Develop a marketable process & catalysts for catalytic upgrading of 2,3-BDO to SAF.
- MFSP  $\leq$  \$2.50 gge with co-product & GHG reduction  $>70\%$

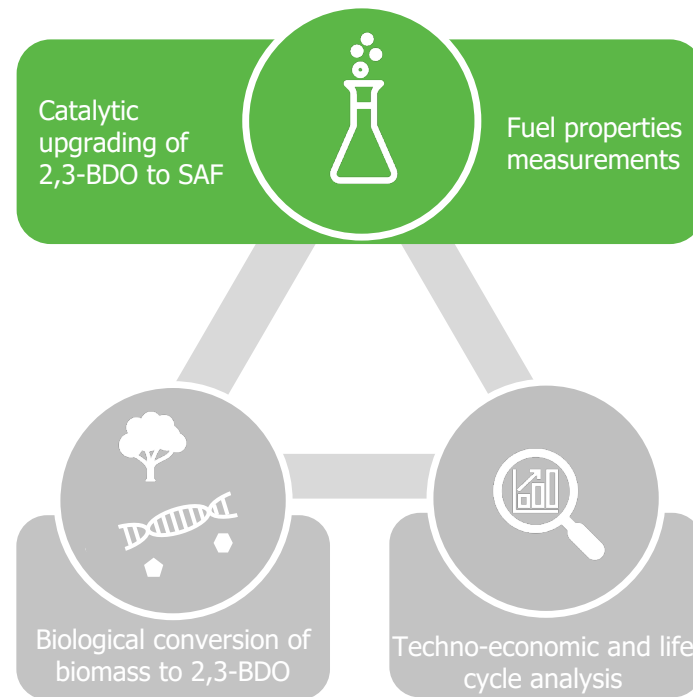
## Approach

- Cohesive integration between upstream biological conversion of biomass to 2,3-BDO fermentation broth with downstream catalytic upgrading of 2,3-BDO to SAF and techno-economic and life cycle analysis

## Relevance

- A hybrid pathway for biomass conversion to SAF to increase the jet fuel blendstock value proposition  $\rightarrow$  BETO goal to decarbonize the aviation sector by 2050

# Catalytic Upgrading of 2,3-butanediol (BDO) to Sustainable aviation Fuels (SAF) Via Methyl Ethyl Ketone (MEK)



# Task Approach

## Novel process

- Operate with aqueous 2,3-BDO: Fermentation broth is 10 wt.% 2,3-BDO/ H<sub>2</sub>O
- No need for energy-intensive separation of 2,3-BDO from water:
  - 2,3-BDO miscible in water
  - 2,3-BDO boiling point (177°C) >> water
  - Separation methods investigated since 1948 ( pilot scale) but not economical yet

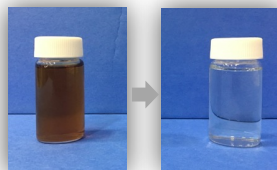
## 2-step approach via MEK

- Convert 2,3-BDO to olefins (SAF precursors) via MEK
- use of metal & mixed oxides catalysts

## Commercially relevant feedstock

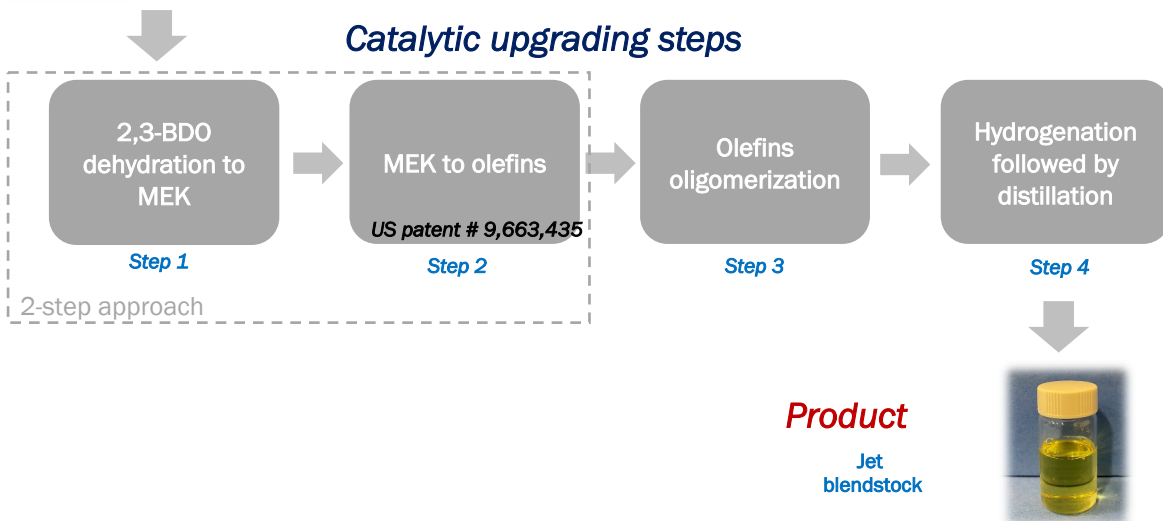
- High titer of 100 g/ Liter
- Pilot scale production demonstrated

# The process for catalytic upgrading of 2,3-butanediol (BDO) to sustainable aviation Fuels (SAF) via Methyl ethyl Ketone (MEK)



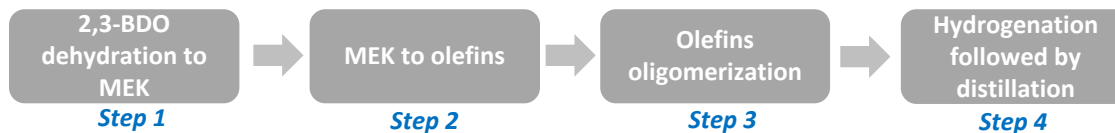
## Feedstock

2,3-BDO fermentation broth  
(100g 2,3-BDO/Liter, ~900g H<sub>2</sub>O)



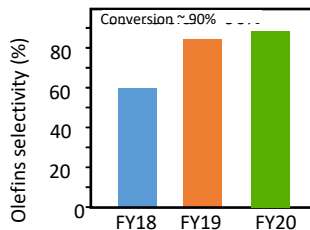


# Progress update for catalytic upgrading of 2,3-BDO to SAF via MEK



## Prior to 2021

- Focus on step 1 & step 2
- Identified preferred catalysts & operating conditions
- **Carbon efficiency improvement coupled with TEA**
- Initiated feedstock composition impact
  - effect of water content in the feed
  - few runs with organic impurities (< 1 wt.%)



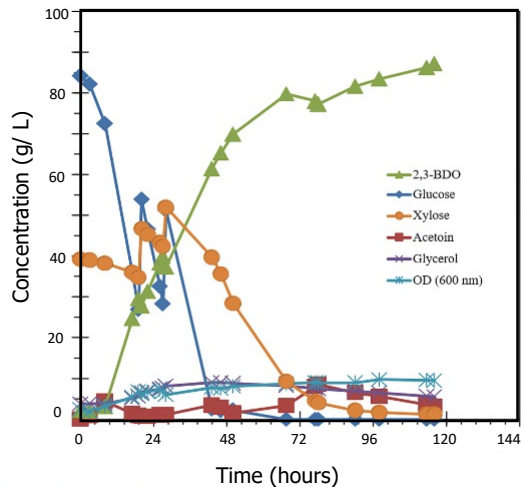
## Since 2021

- **In-Depth study of the impact of the impurities from the real feedstock on the reactivity and catalyst stability**
  - Systematically studied the effect of organic impurities
  - Determined the impact of inorganic K impurity
- **Demonstrated step 1 to 4 and produced SAF for fuel properties measurement**
- **Updated TEA and initiated LCA**
- **Initiated liquid phase upgrading of 2,3-BDO**



# Catalytic performance with the real 2,3-BDO feedstock

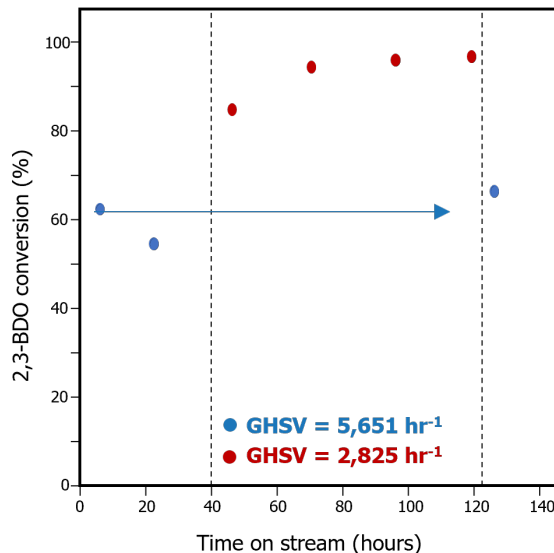
## Pilot scale production of 2,3-BDO fermentation broth



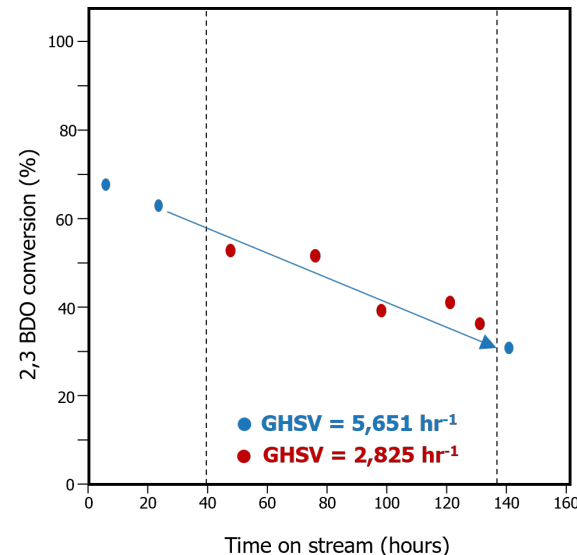
Compound	Pre-filtered 2,3-BDO fermentation broth composition	Post-filtered 2,3-BDO fermentation broth composition
2,3-BDO (wt.%)	9.21	5.45
Acetoin (wt.%)	0.36	0.27
Glycerol (wt.%)	0.60	0.35
Sugars* (wt.%)	2.95	0.02
Acids (wt.%)	0.66	0.00
Proteins (mg/mL)	18.00	0.60
Inorganics: K/Na/S (ppm)	3289/2892/916	429/280/0
Balance is water		

\*mainly cellobiose.

## Model 2,3-BDO Feedstock



## Real 2,3-BDO Feedstock



**Key finding: Deactivation of the catalyst occurs only with the real feedstock containing both organic & inorganic impurities**







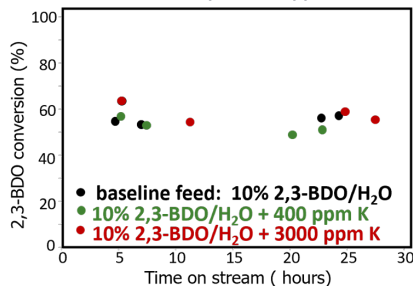
# Progress & outcomes: Demonstrated effect of potassium (K) inorganic impurities from the feedstock on the catalytic performance

## Goal: De-risk potential C efficiency loss due to *inorganic* Impurities

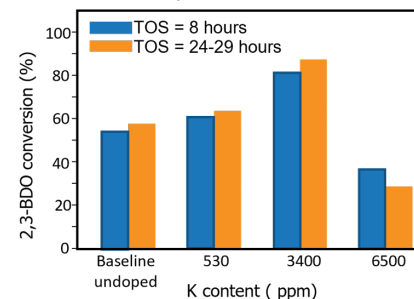
### Technical accomplishments

- Two Approaches:
  - Addition of K to the 2,3-BDO/H<sub>2</sub>O feedstock level: 0, 400, 3000 ppm K
  - Catalyst doping with K for accelerated catalyst aging level: 0, 530, 3400, 6500 ppm K
- Characterization jointly with CDM\* ICP, NH<sub>3</sub>-TPD, TCA
- Addition of up to 3000 ppm K to the 2,3-BDO/H<sub>2</sub>O feedstock does not appear to impact the catalyst performance or its properties.
- Only for the catalyst doped with 6500 ppm K, conversion loss occurs.

The conversion is not impacted by addition of up to 3000 ppm K



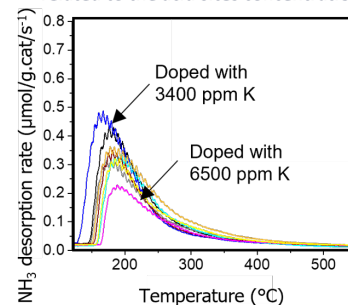
Doping of the catalyst with K impacts the conversion



No detectable change in K level → K did not adsorb on the catalyst

Fresh		139
Spent	●	100
Spent	●	158
Spent	●	154

For K doped catalysts, the conversion is related to the acid sites concentration

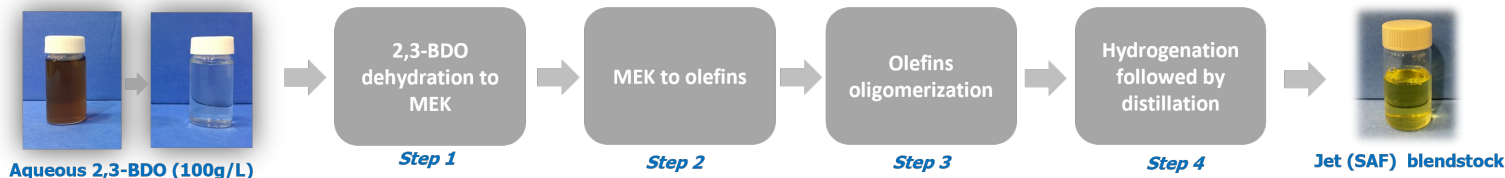


**Key finding:** K impurity from the feedstock can lead to catalyst deactivation after extended time on stream



# Progress & outcomes: 2,3-BDO to SAF blendstock demonstration

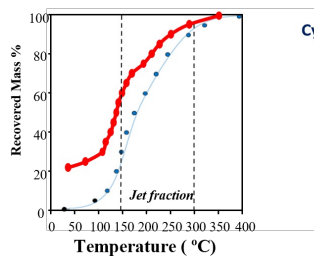
Goal: verify blendstock quality & identify downstream improvements needs



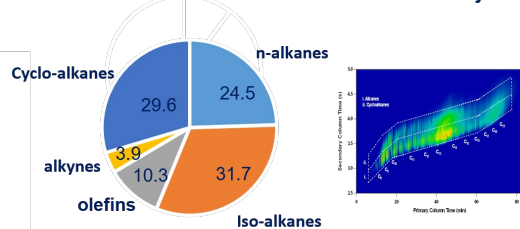
## Technical accomplishments

- Demonstrated each step including distillation
- Oligomerization step ran for 300 hours
- Fuel properties of the recovered jet fuel fraction
  - No blending required

Simulated distillation profile



2D GCxGC molecular structure distribution- jet fraction



**Desired molecular structures :  
(iso)-alkanes and cyclics**

Property	Result	ASTM D7566*
Freezing point (°C)	< -70	Max - 40
Density at 15°C (Kg/m3)	788	775-840
Aromatics (%)	< 0.1	Max 25

\*ASTM D7566 specifications for synthetic paraffinic kerosene

- Oligomerization (step 3): Opportunities for improving per pass conversion & limit recycle
- Hydrogenation (step 4): Need to improve process conditions to ensure complete hydrogenation

**Key finding:** The jet fraction presents promising fuel properties as compared with ASTM D7566 specifications



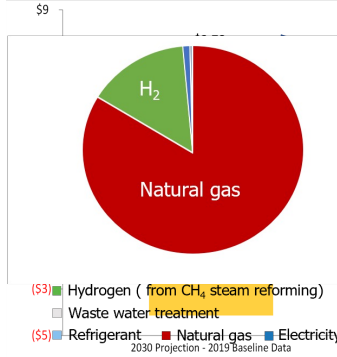
# Progress & outcomes: Updated Techno Economic Analysis (TEA) and initiated Life Cycle Analysis (LCA) of the process

**Goal: Measure progress to achieve MFSP and GHG goals & identify opportunities for improvement**

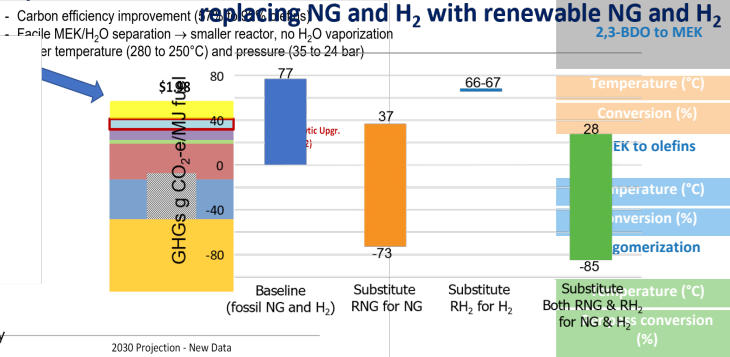
## Technical accomplishments

- Updated TEA
- Conducted preliminary LCA
  - Life cycle inventory : Aspen Plus process model
  - GREET 2021: Carbon intensity for electricity, natural gas (NG), hydrogen (H<sub>2</sub>) and refrigerant (ammonia)

### GHG emissions contributions of the process



### GHG emissions can be greatly reduced when replacing NG and H<sub>2</sub> with renewable NG and H<sub>2</sub>



### Energy impact on minimum fuel selling price

Parameter	2019 SO	2019 SO update	2021 SO update	2022 SO update
MFSP (\$/GGE)	\$3.00	\$2.85	\$2.44	\$2.48
Temperature (°C)	280	280	\$2.44	\$2.48
Conversion (%)	>99	>99	>99	>99
Temperature (°C)	400	400	400	400
Conversion (%)	90.1	97.7	97.7	97.7
Temperature (°C)	220	220	220	220
Conversion (%)	41%	41%	41%	41%

**Key finding: Natural gas is the main contributor to the GHG emissions due to water vaporization**

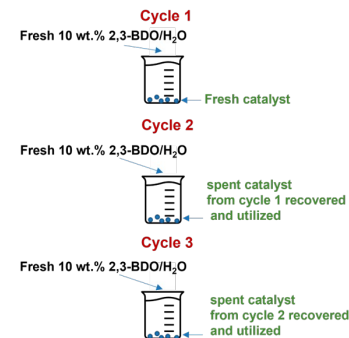
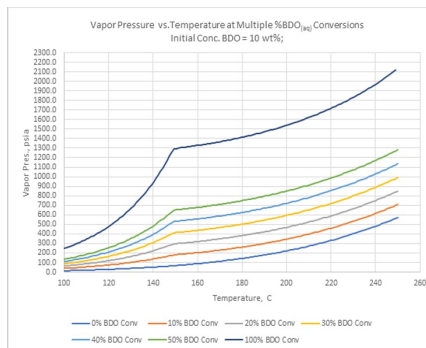


# Progress & outcomes: Introduced liquid phase upgrading of 2,3-BDO to MEK to reduce GHG emissions

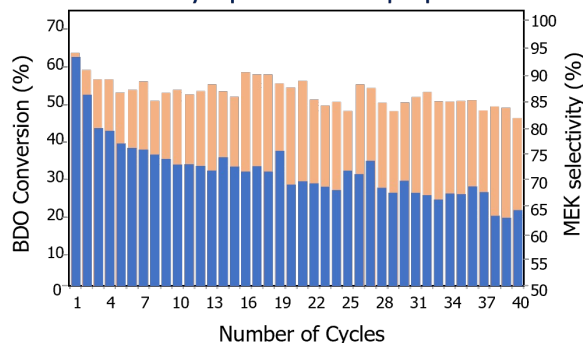
**Goal: Evaluate potential of liquid phase upgrading of 2,3-BDO for GHG reduction**

## Technical accomplishments

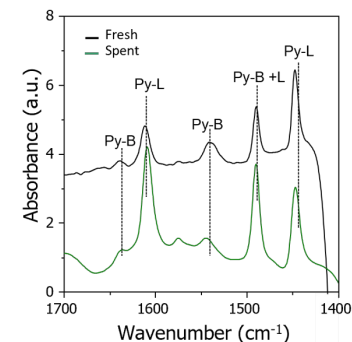
- Catalysts screening
  - 3 different types of catalyst
- Multiple cycles in batch reactor
  - T = 200°C, P = 1550 psig
  - 10 wt.% 2,3-BDO/H<sub>2</sub>O
- Characterization jointly with CDM
  - 6 techniques for surface and structure properties  
XRD, NH<sub>3</sub>-TPD, ICP, Pyridine FT-IR, N<sub>2</sub> adsorption/ desorption
- Modes of deactivation identified for several catalyst families: coking, loss of crystallinity, loss of acid sites
- Successfully demonstrated 40 continuous cycles



Multiple cycles conducted to test the catalysts performance in liquid phase



FT-IR pyridine of fresh and spent catalysts



**Key finding: Liquid phase upgrading of 2,3-BDO to MEK appears feasible**



# Summary of key accomplishments, outcomes and impact since 2021

## Technical progress & Outcomes since 2021

### ➤ Met Go/ no Go & achieved all 6 milestones

- Demonstrated 65% in MFSP cost reduction for catalytic upgrading compared to 2019 SOT
- 5 milestones in collaboration with CDM, ACSC, TEA/LCA teams

### ➤ Advanced understanding of the 2,3-BDO feedstock requirements

- Identified which impurities from the 2,3-BDO fermentation broth will impact the catalyst performance and to what level.
- Guide activities related to fermentation broth production and conditioning prior to catalytic upgrading of 2,3-BDO fermentation broth

### ➤ 2,3-BDO to SAF process demonstration

- Demonstrated each step of the process, produced jet fuel and measured the fuel properties following ASTM D7566 criteria

### ➤ Initiated LCA that identified natural gas as the main contributor to GHG and help understand how to reduce GHG emissions

## Impact since 2021

### ➤ Results Dissemination

- 1 new publication in FY22  
<https://doi.org/10.1016/j.fuel.2022.126328>
- Regularly attend & present at ACS and NAM conferences

### ➤ New market opportunity

- International recognition in the field led to 1 new CRADA project with 500 fortune company to investigate upgrading of another biologically-derived diol

### ➤ Stakeholder engagement

- Attended and presented work concerning impurities at the 2,3-BDO summit held by DOE-BETO
- Attend bi-weekly ChemCatBio (CCB) meetings, annual all-hands (CCB) meetings & monthly CUBI meeting

### ➤ Enhanced value proposition of hybrid processes for conversion of biomass to SAF via 2,3-BDO intermediate

- Experimental work combined with TEA & LCA contribute to improve value proposition and minimize risks

# 2,3-BDO Upgrading via Dioxolane Intermediates

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Xiaokun (Claire) Yang, LANL

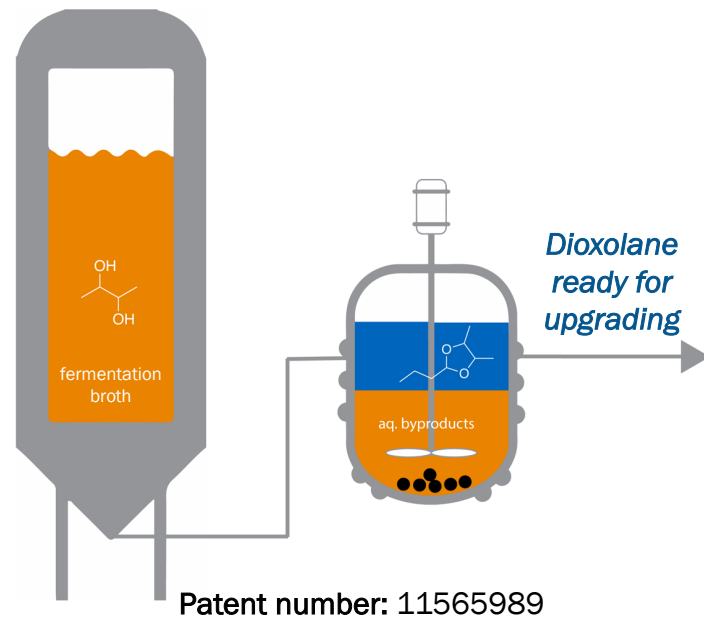
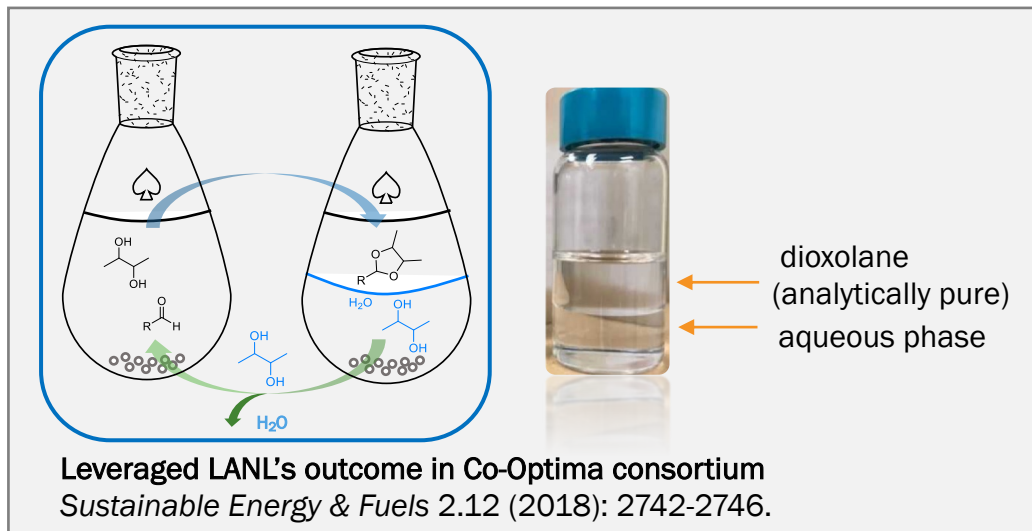
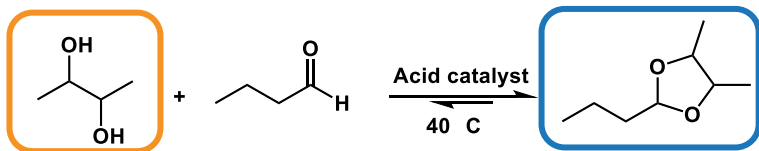






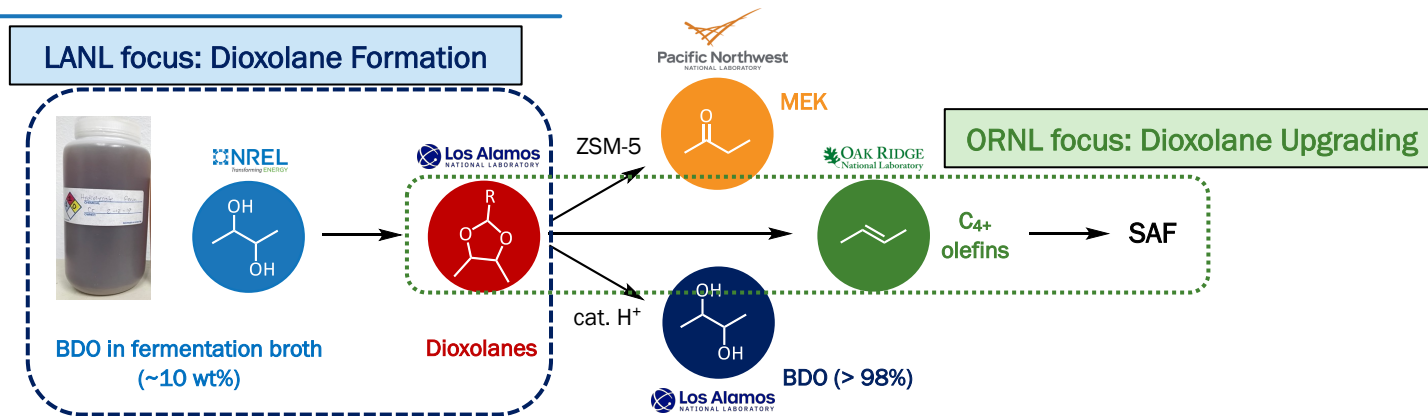
# Overview: 2,3-BDO Upgrading via Dioxolane Intermediates

**Objective:** upgrading fermentation-derived 2,3-butanediol (BDO) into sustainable aviation fuel (SAF) with a distillate MFSP of \$2.50/GGE or less and GHG emissions reduction at 70% or more via dioxolane pathway





# Approach: Dioxolane as a Versatile Platform Chemical



## Prior to 2021

- Dioxolane formation in **real fermentation broth**
- **Catalyst lifetime** increasing
  - Pre-treating fermentation broth with ion-exchange resin
- Dioxolane upgrading to **MEK**
- **2,3-BDO recovery** via dioxolane intermediate

## Since 2021

- **Produced dioxolanes** with various aldehydes and ketones
  - Chain length and structure effect
  - **Renewably sourced** aldehydes
- **Delivered broth-based dioxolanes** to ORNL for catalytic upgrading
- **Further reduced MFSP and GHG emission**
  - Butyraldehyde consumption reduction
  - New catalyst development
  - **Initiated TEA guided process integration**

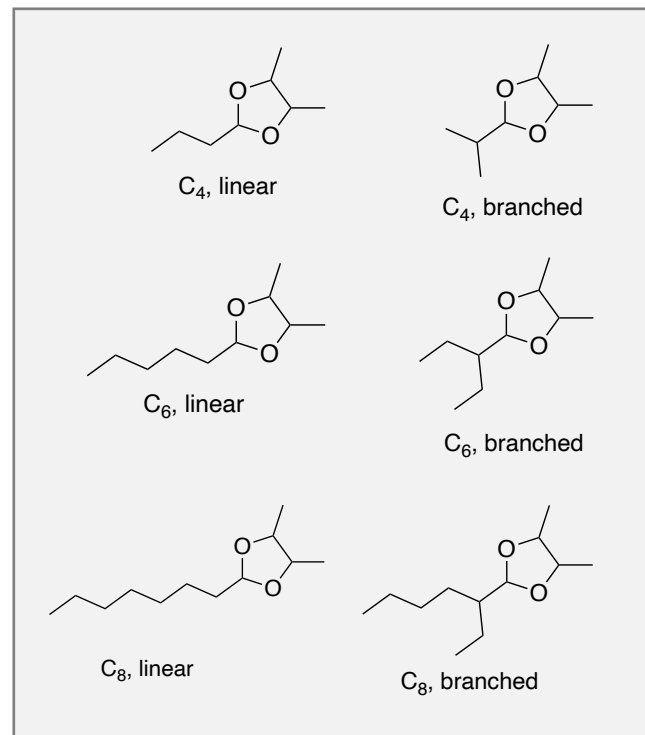


# Progress & Outcomes: Formation of Multiple Dioxolanes

**Objective:** testing dioxolanes formation with different tailing structures

- ✓ Dioxolanes synthesized from **C<sub>4</sub>**, **C<sub>6</sub>**, and **C<sub>8</sub>** aldehydes with different chain lengths and branches
- ✓ 6 dioxolanes with **linear or branched structures** were synthesized **in large scale**
- ✓ Delivered 50 mL of each sample to ORNL for downstream upgrading
- ✓ Delivered >20 mL dioxolanes with NREL fermentation broth to ORNL for upgrading

**Key Finding:** Both linear and branched dioxolanes we tested can be produced in aqueous solutions with phase separation, avoiding energy-intensive BDO-water separation



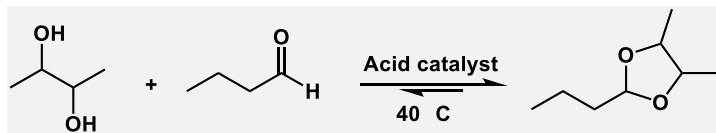
\* *Dioxolanes themselves exhibit good to excellent combustion properties as diesel fuels*



# Progress & Outcomes: Aldehyde Consumption Reduction

**Objective:** Reduce the consumption of fossil-based butyraldehyde to potentially reduce the energy input and overall cost

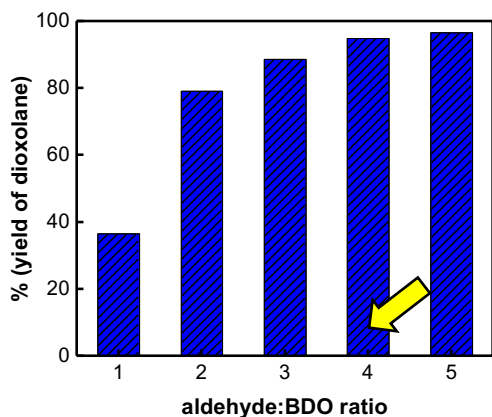
Tested with aq. BDO (79 g/L)



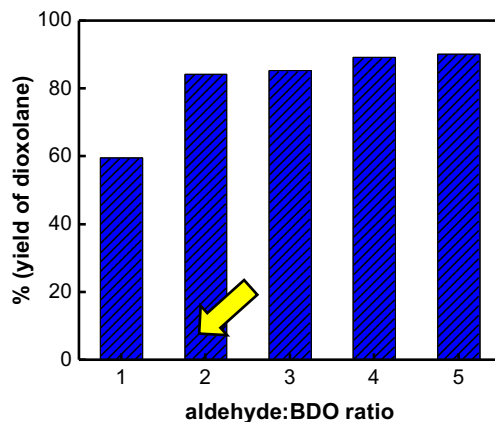
1 eq.

5 eq.

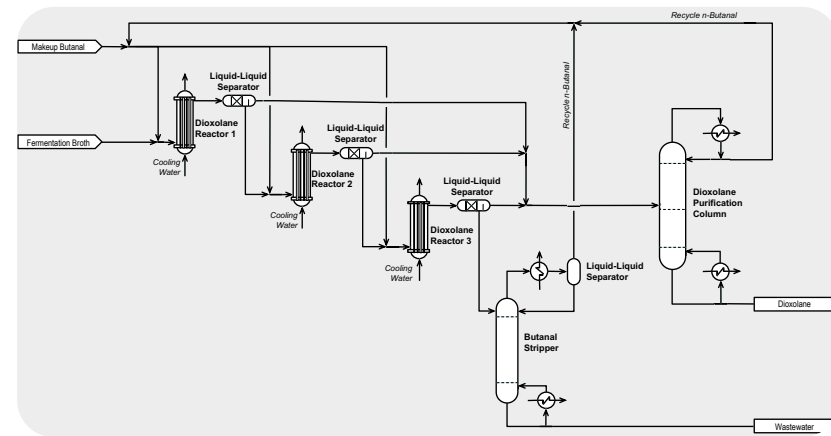
Amberlyst-15



Nafion NR50



## 3-stage reactive extraction by Separation Consortium


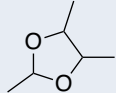
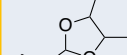
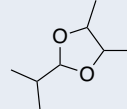
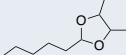
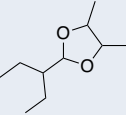
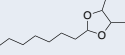
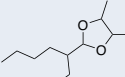
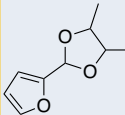
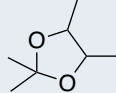
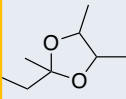


**Key Finding:** The current 5 eq. of butyraldehyde to BDO loading can be reduced to ~1.4 eq. with a 3-stage reactive extraction in large scale



# Progress & Outcomes: Renewably Sourced Dioxolanes

**Objective:** Experimentally synthesize dioxolanes from BDO and renewably sourced aldehydes/ketones to study for additional dioxolane conversion studies

Aldehyde or Ketone	Formaldehyde	Acetaldehyde	Butyraldehyde	Isobutyraldehyde	Hexaldehyde	2-Ethylbutyraldehyde	Octaldehyde	2-Ethylhexaldehyde	Furfural	Acetone	Methyl Ethyl Ketone
Short Name	C <sub>1</sub>	C <sub>2</sub>	C <sub>4</sub> , linear	C <sub>4</sub> , branched	C <sub>6</sub> , linear	C <sub>6</sub> , branched	C <sub>8</sub> , linear	C <sub>8</sub> , branched	C <sub>furan</sub>	C <sub>dimethyl</sub>	C <sub>methyl-ethyl</sub>
Molecular Structure											

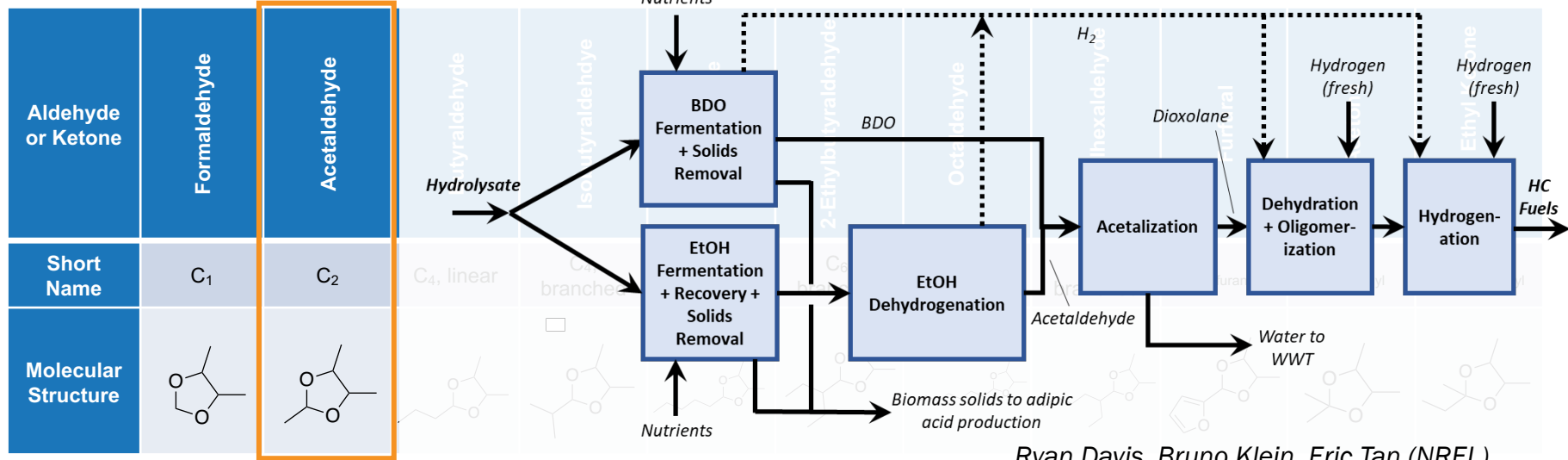
- ✓ Dioxolanes formed with a wide range of aldehydes/ketones that can be renewably sourced
- *Ketone-derived dioxolanes cannot be prepared in water due to reaction equilibrium*

Delivered ~ 40 mL renewably sourced dioxolanes to ORNL for catalytic upgrading



# Progress & Outcomes: TEA/LCA Guided Process Integration

**Objective:** Initiate process integration for BDO upgrading via dioxolane intermediate to potentially lower GHG emission

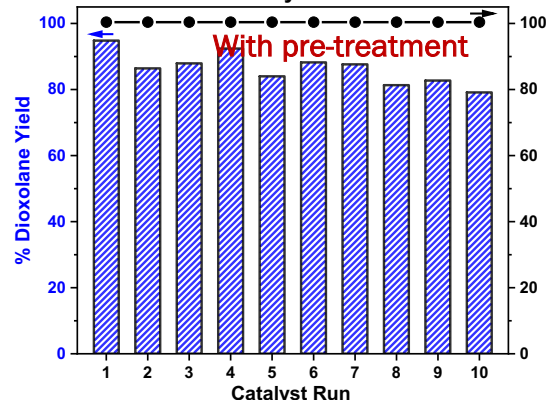
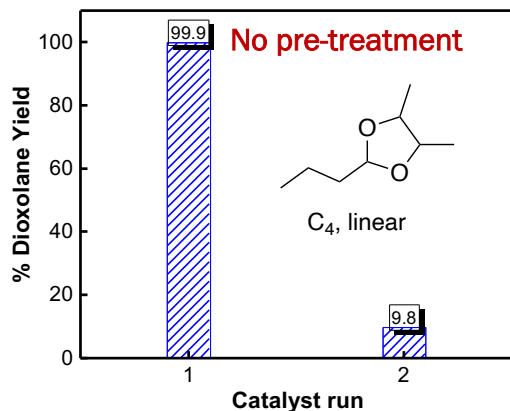


**Key Finding:** Processes integration of BDO upgrading with EtOH production via the dioxolane pathway can potentially save both capital and operational cost, combined impacts can achieve >70% GHG reduction threshold



# Progress & Outcomes: Catalyst Stability Examination

**Objective:** Increase catalyst lifetime in real fermentation broth



## Inorganic impurities

Sample/Metals	K ppm	Na ppm	Ca ppm	Mg ppm
Hydrolysate broth	3357	1905	141	83
Hydrolysate broth after <b>Nafion NR50</b> treatment	2350	1588	87	71
Hydrolysate broth after <b>Amberlyst-15</b> treatment	252	326	4	1
Hydrolysate broth after <b>ion-exchange resin*</b> treatment	ND	ND	ND	ND

\*Dowex 50WX8

## Organic impurities

Compound	Hydrolysate broth (g/L)
<b>2,3-BDO</b>	79.1
Glucose	1.4
Xylose	2.0
Arabinose	6.0
Acetoin	3.3
Glycerol	5.1
Xylitol	1.0
Lactic acid	2.0
Ethanol	0.8
Acetic acid	1.5

- Amberlyst-15 and Nafion NR50 are resin catalysts that can be deactivated by metal ions in the broth
- Ion-exchange resin can remove metal ions and increase catalyst lifetime
- Organic impurities are mainly remained in aqueous broth and less pre-treatment will be required for the dioxolane pathway.

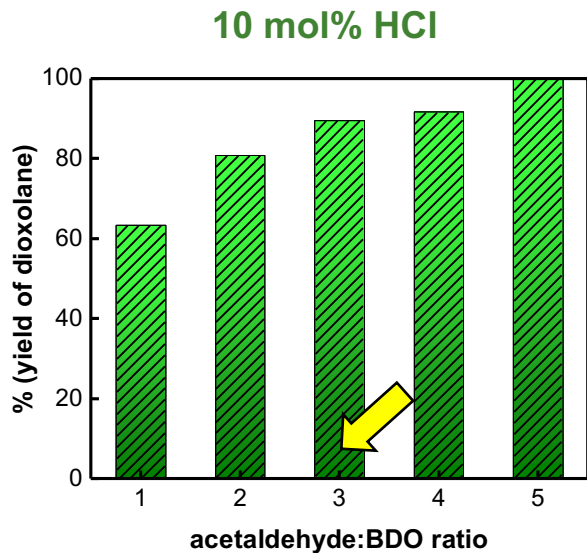
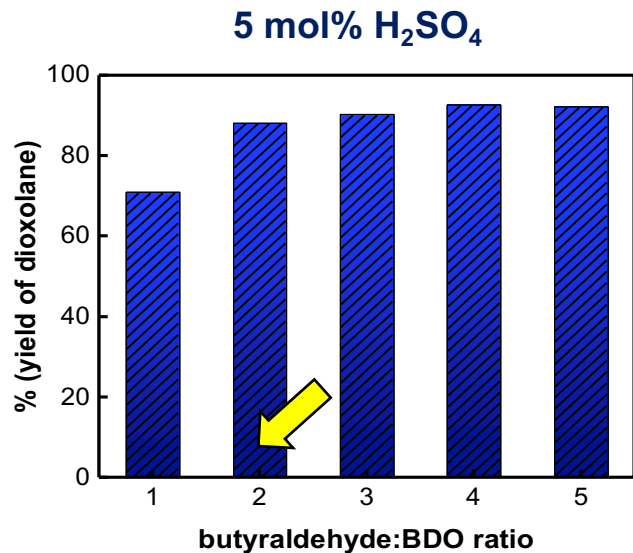




# Progress & Outcomes: New Catalyst Development

**Question:** Eliminate the pre-treatment step and use mineral acid as catalyst for dioxolane formation?

*Ion exchange resin column regeneration requires HCl*



**Dilute mineral acid catalyst:**

- ✓ No need for ion-exchange resin column regeneration
- ✓ High BDO conversion and dioxolane yield
- ✓ Low aldehyde consumption
- ✓ Good phase separation

**Potential positive impact on capital and operational cost and GHG reduction**



# Summary of key outcomes and impact since 2021

## Progress & Outcomes since 2021

- Achieved all **3 technical milestones**
- Evaluated dioxolane synthesis via renewably sourced aldehydes and ketones
- Delivered **> 300 mL dioxolanes samples** to ORNL to evaluate dioxolane downstream upgrading
- **Achieved >70% GHG reduction** threshold with process integration for BDO upgrading via dioxolane pathway (**by TEA/LCA**)
- On track to new milestone on developing strategies to recover and recycle aldehydes from dioxolanes for process cost reduction

## Impact since 2021

- 1 new **publication** in 2023
- 1 new **patent** application
- Regularly attend & present at AIChE and GCE **conferences**
- Stakeholder engagement
  - Bi-weekly ChemCatBio (CCB) meetings
  - Annual all-hands (CCB) meetings
  - Monthly CUBI meetings

# 2,3-BDO Upgrading via Dioxolane Intermediates

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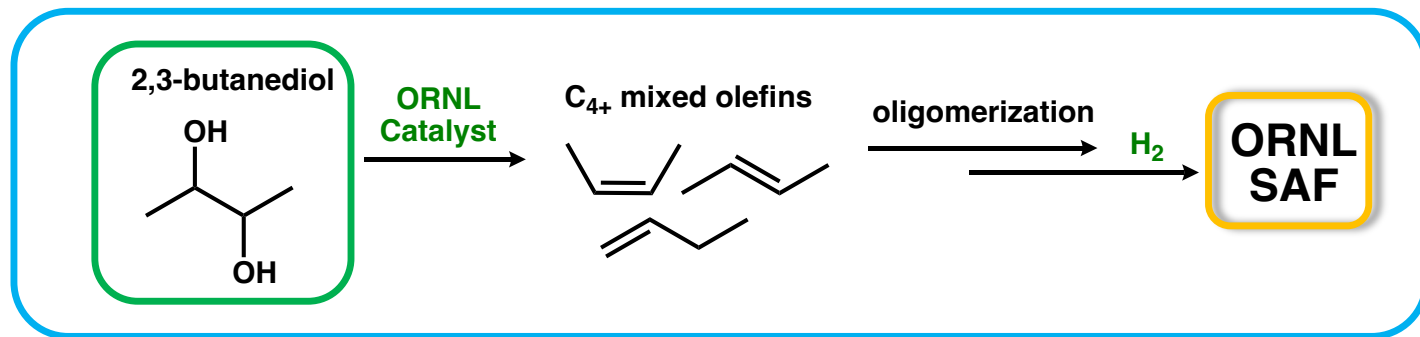
Andrew Sutton, ORNL





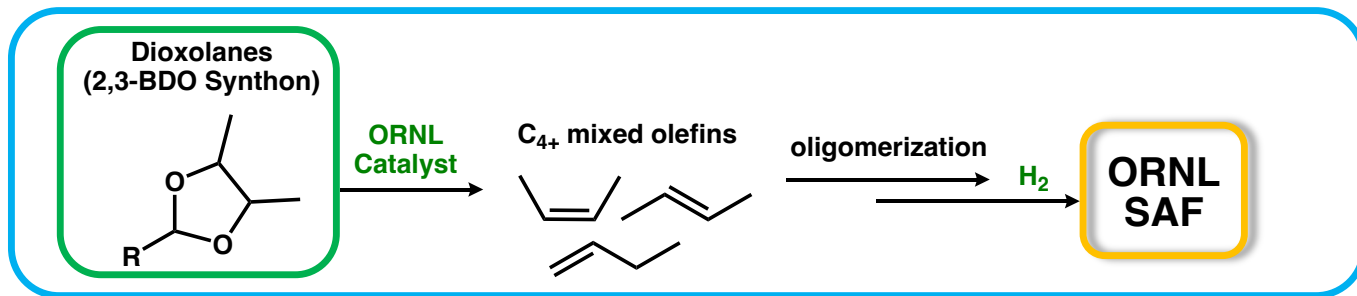
# Task Overview

De-risk 2,3-butanediol (BDO) upgrading processes to SAF to enable technology for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions of <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of a reasonable fuel MFSP (i.e., ~\$2.50/gge)





# Overview – ORNL Approach to Convert Dioxolanes to SAF



**Prior work:** Develop catalyst technology to produce middle distillate and chemical coproducts from biomass-derived 2,3-BDO

- One step highly selective production of C<sub>3</sub>-C<sub>6</sub> olefins in high yield with co-production of methyl ethyl ketone (MEK)
- Cu/Pillared-MFI can reduce coke formation by >50% for BDO conversion to olefins

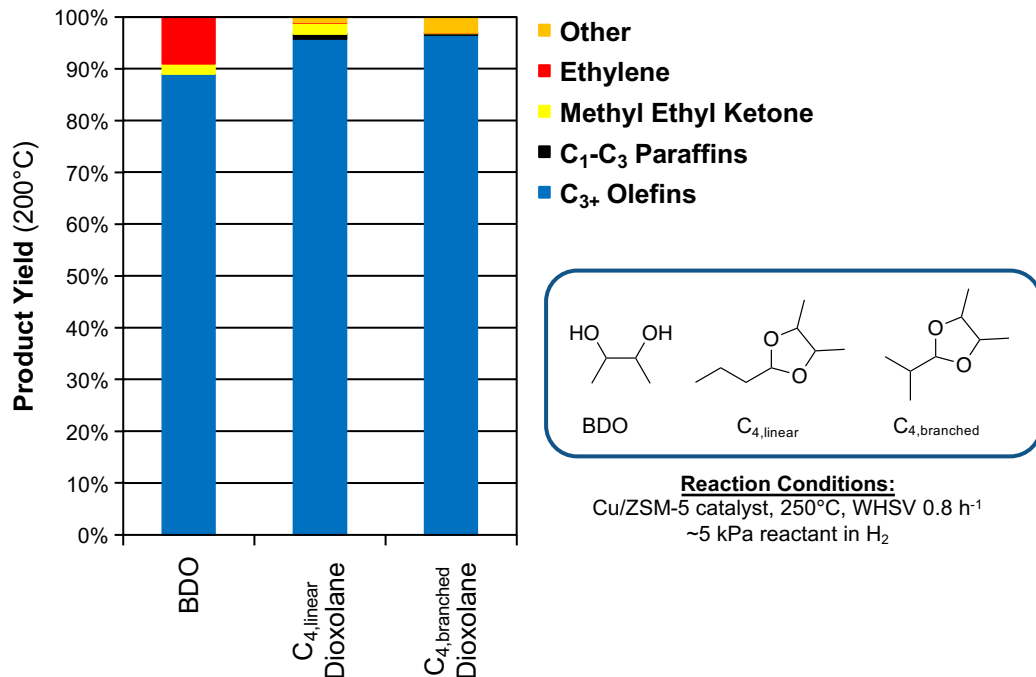
**New Goal:** Adapt BDO conversion approach to utilize dioxolanes as BDO synthon

- Dioxolanes have potential reactive separation benefits for BDO recovery from fermentation broth
- Potential for overall reduced CapEx and OpEx
- Are dioxolanes interchangeable with BDO?
- Can aldehyde be recovered and recycled, or can that be incorporated into the final olefin product to offer a performance advantage?



## 2. Progress & Outcomes: BDO vs Dioxolanes

**Goal:** Demonstrate dioxolane conversion to olefins over Cu/ZSM-5 relative to pure BDO



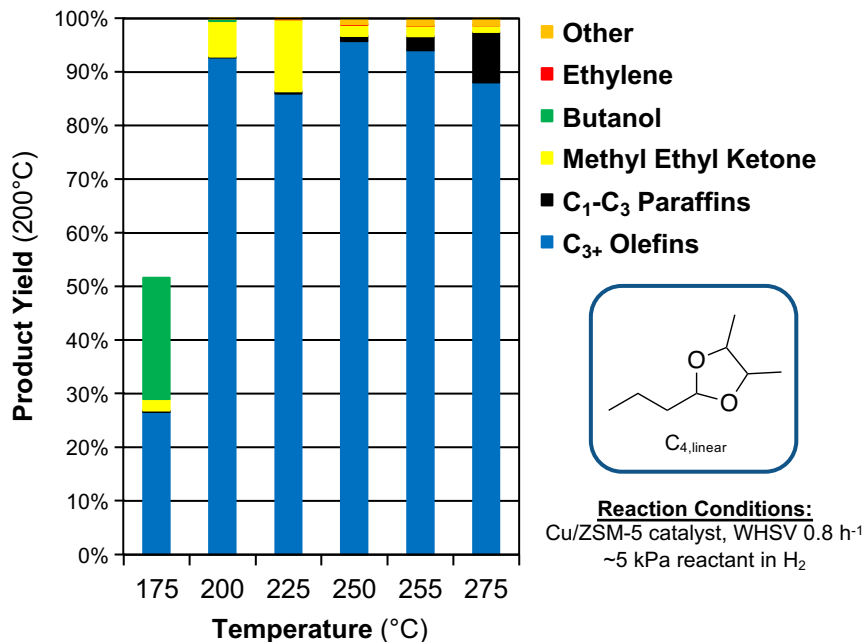
- Use of dioxolanes for efficient BDO separation provides opportunity for direct conversion without BDO recovery
- Eliminates water heating and hydrothermal stability requirements
- Exceeds C<sub>3+</sub> olefin (alkenes) selectivity under identical reaction conditions (>95%)

**Dioxolanes are interchangeable with BDO and also provide improved conversion to C<sub>3+</sub> olefin relative to BDO**



## 2. Progress & Outcomes: Dioxolane Conversion with Temperature

**Goal:** Demonstrate temperature effects on dioxolane conversion and olefin formation



- Below 200 °C incomplete hydrogenation and dehydration is observed
- Using existing catalyst platform gives high conversion and C<sub>3+</sub> olefins selectivity
- Higher olefin distributions changes with temperature
- Increasing temperatures yields paraffin (alkanes) formation, decreasing olefin (alkene) yields.

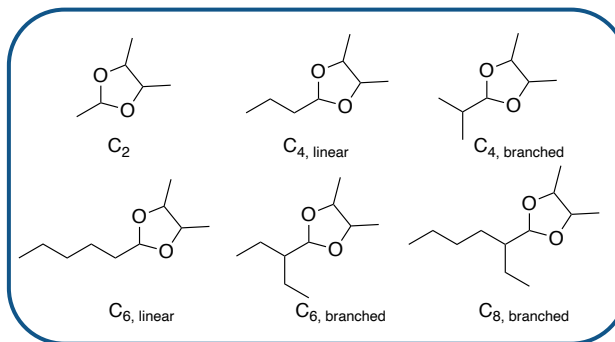
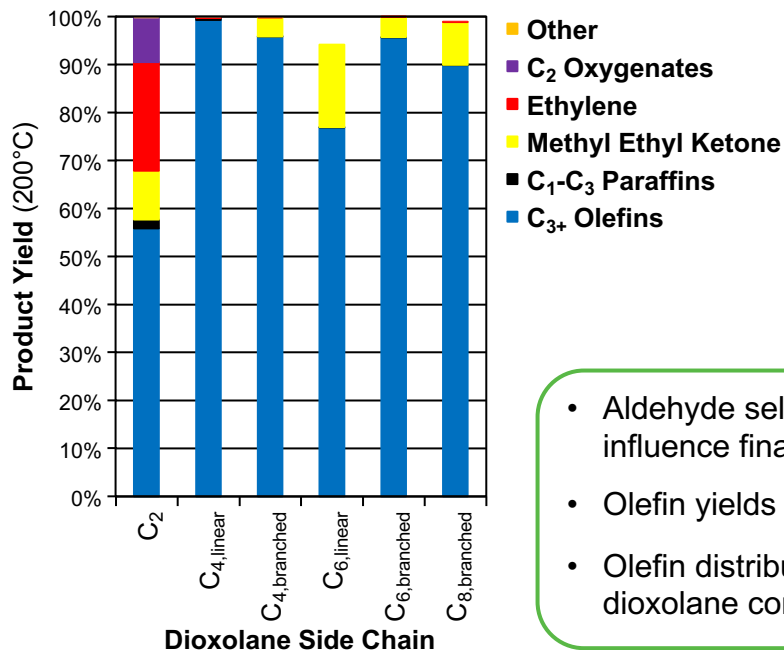
- **100 % conversion and >95% C<sub>3+</sub> olefin selectivity achievable via dioxolane conversion**
- **Temperature “sweet spot” identified for maximizing olefin and minimizing paraffin formation**





## 2. Progress & Outcomes: Dioxolanes from Varied Aldehydes

**Goal:** Demonstrate effect of aldehyde selection on olefin distribution



**Reaction Conditions:**  
Cu/ZSM-5 catalyst, 225°C,  
WHSV 0.8 h<sup>-1</sup>  
~5 kPa reactant in H<sub>2</sub>

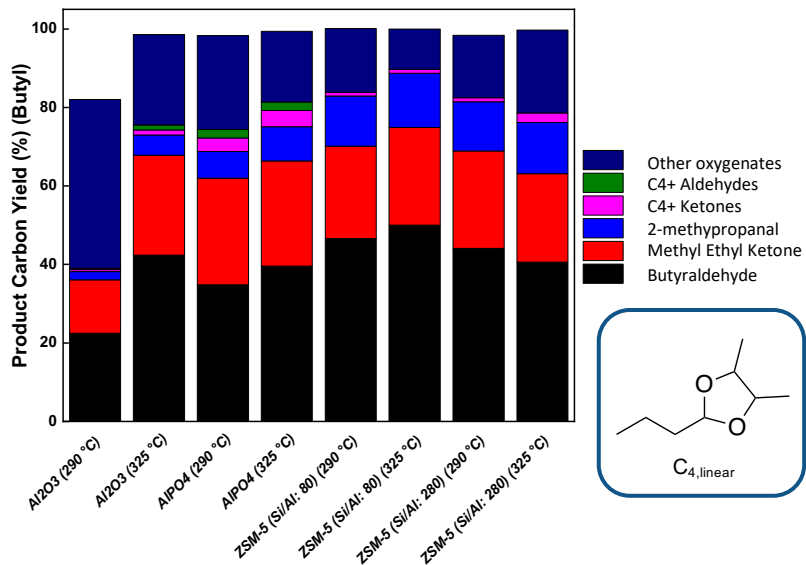
- Aldehyde selection may impact separations behavior or olefin distribution to influence final fuel properties
- Olefin yields remain high regardless of parent aldehyde carbon chain length
- Olefin distributions reflect both BDO- and aldehyde-derived components from dioxolane conversion

**100 % conversion and >95% olefin selectivity achieved from multiple dioxolane compounds**



## 2. Progress & Outcomes: Aldehyde Recovery

**Goal:** Demonstrate potential for aldehyde recycle from dioxolane conversion pathways



*In collaboration with Karthi Ramasamy at PNNL*

- FY23 Q2 milestone focuses on aldehyde recovery and recycle
- Near quantitative recovery of aldehyde is possible
- Hydrogen partial pressure also influences recovery
- Potential for overall process intensification to further improve TEA and LCA

**Recovery of aldehydes for recycle in the overall process has been demonstrated in quantitative yield**



## 2. Progress & Outcomes: Improvements

	FY21 (BDO)	FY23 (BDO)	FY23 (Dioxolane)	Target
<b>Catalyst</b>	Cu/PMFI	Cu/ZSM-5	Cu/ZSM-5	Improved Design
<b>Process Conditions</b>	250 °C 1 atm 99 kPa H <sub>2</sub>	250 °C 1 atm 99 kPa H <sub>2</sub>	200-250 °C 1 atm 0-99 kPa H <sub>2</sub>	200 °C 1 atm H <sub>2</sub> 50 kPa
<b>BDO Feed</b>	BDO	BDO	Dioxolane	Fermentation Derived Optimized Dioxolane
<b>Feed Single-pass Conversion</b>	100%	100%	100%	100%
<b>C<sub>3+</sub> Olefin Selectivity</b>	>95%	>88%	> 97%	> 97%
<b>Ethylene Selectivity</b>	<5%	9%	< 1%	< 1%
<b>GHG &amp; MFSP</b>	\$7.79 GGE	-	\$2.53 GGE 62% GHG reduction relative to petroleum (market-value allocation)	TBD



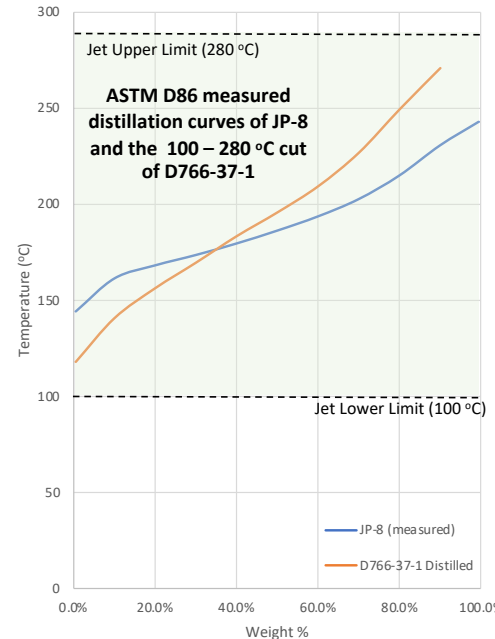
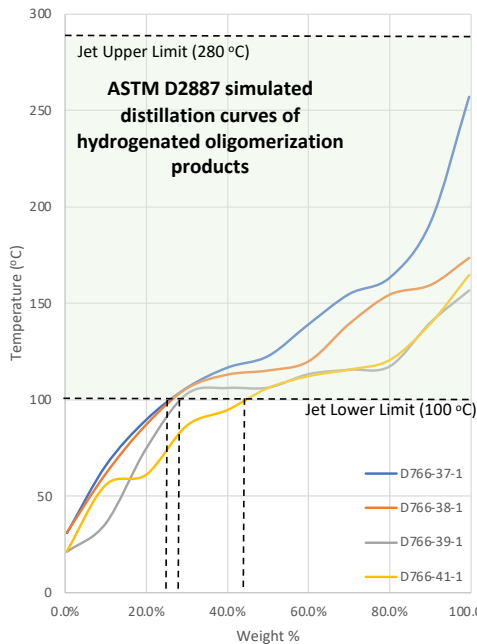
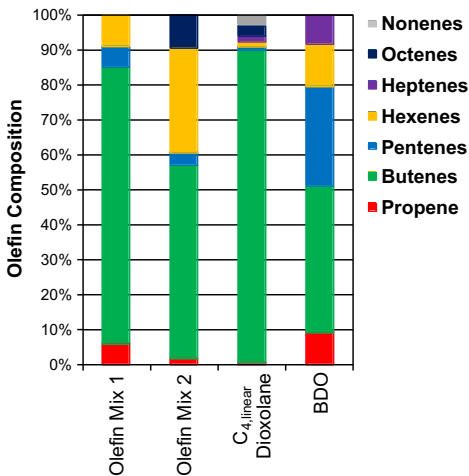
## 2. Progress & Outcomes: Future R&D

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- **Optimize operating conditions and increase time on stream to > 500 hrs**
- **Understand possible deactivation pathways and develop catalyst regeneration protocol**
- **Develop the use of engineered catalysts (e.g. extrudates and pellets) (with ACSC)**
- **Improve catalyst selectivity and stability for C<sub>4+</sub> rich olefin streams (with CDM)**
  
- **FY23-Q3: Develop strategies to recover and recycle aldehydes from dioxolanes**
  - Lowering the process cost of BDO to olefins via dioxolane pathway by investigating aldehyde recovery solutions to decrease process costs from significant aldehyde feed requirements during aqueous dioxolane formation.
- **FY24 Go/No-go: Carbon Efficiency of Oligomerization Processing Step to Meet Economic Targets**
  - Achieve at least 80% carbon efficiency for single step oligomerization of produced olefins to SAF range hydrocarbons using an engineered catalyst. If unsuccessful evaluate the use of more complex and costly multi-step oligomerization technology.
- **End of Project Goal (FY25): De-risk biochemical intermediate upgrading processes to SAF to enable technology for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions of <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of a reasonable fuel MFSP (i.e., ~\$2.50/gge).**



# 3. Impact: Product Chemistry Well Suited for SAF



Olefin Mix 1	Sample	Catalyst	Temp (°C)	Time (hr)	Scale (g)	Carbon Balance
	D766-37-1	Amberlyst-36	150	11	70	98.5%
Olefin Mix 2	D766-39-1	ZSM-5	200	11	35	70.0%
	D766-41-1	Beta Zeolite	200	11	35	66.5%
Olefin Mix 2	D766-38-1	Amberlyst-36	150	11	30	85.0%

- Olefin surrogate mixtures oligomerized and hydrogenated in batch reactors
- Near quantitative conversion to isoalkanes
- Complete conversion of C<sub>3</sub>'s
- Excellent jet conversion
- 100% with recycle of lights

Fuel Type	Freezing Point (°C)	Flash Point (°C)	Viscosity @ -20 °C (mm <sup>2</sup> /s)	Cloud Point (°C)	Density @ 15 °C (g/cm <sup>3</sup> )	Energy Density (MJ/L)	Specific Energy (MJ/kg)
ORNL SAF (D766-37-1 Distilled)	< -65	32.5	4.778	< -65	0.7743	46.5	36.0
Jet-A	< -40	>38	< 8	-	0.775-0.840	42.7	34.0



# Project Level Impact

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# Project Level Summary and Conclusions

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# Acknowledgements

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# Acknowledgements

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Hydrolysis Project  
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Prof. Sunkyu Park  
David Cruz Rios  
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# Acknowledgments-MERGE at end

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# Acknowledgments to add to common slides with other tasks

---

## *CUBI Team (PNNL)*

Vanessa Lebarbier Dagle

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Teresa Lemmon

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Aye Meyer



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---



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TEA Analysis  
NREL



**Steve Phillips**  
TEA Analysis  
PNNL

# Thank You!

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[chemcatbio.org](http://chemcatbio.org)

*This work was performed in collaboration with the Chemical Catalysis for Bioenergy Consortium (ChemCatBio, CCB), a member of the Energy Materials Network (EMN)*

# Appendices

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[chemcatbio.org](http://chemcatbio.org)

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# Extra Slides

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*This work was performed in collaboration with the Chemical Catalysis for Bioenergy Consortium (ChemCatBio, CCB), a member of the Energy Materials Network (EMN)*

# Quad Chart Overview

## Timeline

- Project start date
- Project end date

	FY22 Costed	Total Award
DOE Funding	(10/01/2021–9/30/2022)	(negotiated total federal share)
Project Cost Share*		

TRL at Project Start:

TRL at Project End:

## Project Goal

Include a concise, clear project goal statement (examples in notes section).

## End of Project Milestone

Add your end of project technical target/milestone per your SOPO or AOP.

## Funding Mechanism

Which FOA or Lab Call, topic area, and year, if applicable.

## Project Partners\*

- Partner 1
- Partner 2

*\*Only fill out if applicable.*



# Catalytic Upgrading of Biochemical Intermediates (CUBI) – Overall Project

Jeff Linger, Jake Miller & David Johnson (NREL), Andrew Sutton (ORNL), Vanessa Dagle (PNNL), Xiaokun Yang (LANL)

WBS# - 2.3.1.101-104

**Project Objectives.** FY23-25 CUBI work will focus on de-risking and optimizing catalytic processes to support commercialization efforts for our promising portfolio of SAF pathways while leveraging core ChemCatBio capabilities. This project will focus on upgrading fermentation-derived carboxylic acids (NREL), fermentation-derived 2,3-BDO (PNNL, ORNL, LANL), and sugar-derived furans (NREL) into sustainable aviation fuel.

**Technical Approach** (*see individual task charts for specifics*): Broadly, this project seeks to lower process costs and increase efficiency in novel catalytic upgrading approaches of intermediates derived from biogenic sources into sustainable aviation fuel.

## Project Milestones and Outcomes

- Starting TRL and Ending TRL: TRL3→TRL4
- End of project goal/milestones: De-risk end-to-end biochemical intermediate upgrading processes to SAF...demonstration of life-cycle GHG emissions targeting <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.
- Go/No-Go's w/date: Each Task has an independent Go/No-Go milestone

## Decarbonization Pillars and EERE Emphasis Areas

- The Catalytic Upgrading of Biological Intermediates (CUBI) project directly focuses on establishing and scaling technologies to produce sustainable aviation fuel from biogenically sourced intermediates thus **decarbonizing the transportation sector**.
- The ChemCatBio consortium as a whole is dedicating efforts towards Diversity, Equity and Inclusion activities. While activities are currently unspecified, these will be adopted and pursued by the CUBI project (**Diversity in STEM**).

## Project Attributes

Project Start and End Dates	10/1/2022-9/30/2025	
FY23 Budget	Total: \$1350K (NREL), \$400K (ORNL), \$450K (PNNL), \$250K (LANL)	
Collaborations	ChemCatBio – CUBI	See individual task quad charts
DOE TM Lead	Sonia Hammache	Sonia.Hammache@e.e.doe.gov

# CUBI—Carboxylic Acids

Jacob Miller (NREL)

2.3.1.101

## Project Objectives

In support of CUBI, this task aims to upgrade short-chain fermentation-derived carboxylic acids (primarily C4 butyric acid) to sustainable aviation fuel.

## Technical Approach

- Focus on expanding the portfolio of available carboxylic acid upgrading technologies through development of novel light acid upgrading pathways in FY23
- Develop continuous catalytic processes for upgrading of C<sub>2-4</sub> acids into jet-range branched and cyclic hydrocarbons
- Run promising upgrading processes for at ~100 hours on stream to assess catalyst stability

## Project Milestones and Outcomes

- Starting TRL: 3; Ending TRL: 4
- FY22 Q4 SMART milestone: We will screen catalysts for butyric acid upgrading to jet-range (C8-16) branched, cyclic, and aromatic hydrocarbons and oxygenates in flow reactors. Feed butyric acid and/or 4-heptanone over at least four solid oxides (e.g., TiO<sub>2</sub>, niobic acid, H/ZSM-5) and determine at least one set of reaction conditions (pressure, temperature, WHSV) sufficient to obtain at least 40% carbon yield of jet-range branched, cyclic, and/or aromatic hydrocarbons and oxygenates. Run upgrading for at least 100 hours on stream, also achieving at least 40% carbon yield of jet-range compounds with a WHSV greater than 0.1 hr<sup>-1</sup>. Then, hydrotreat upgraded molecules to show at least 20% carbon yield of jet-range compounds from acid feed to hydrocarbon product. Data will be reported to NREL's Analysis Group for consideration in the Biochemical SOT.
- FY23 Q2 Go/No-Go: We will convert biogenically-sourced butyric acid into to 100 mL sustainable aviation fuel blendstock through demonstration of each process step targeting an overall process carbon yield of 60%. Report findings to projects focusing on upstream biological processes to align SOT-relevant research targets and determine whether upgrading of bio-butyric acid creates products most suitable for SAF or other (e.g., chemicals) applications.
- End-of-project milestone: De-risk end-to-end biochemical intermediate upgrading processes to SAF to clearly articulate cases for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions targeting <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.

## Project Attributes

Project Start and End Dates	October 1, 2022 – September 30, 2025	
FY23 Budget	Total: \$459 K	
Collaborations	CCPC 2.5.1.302	<a href="mailto:assary@anl.gov">assary@anl.gov</a> (630) 252-3536
DOE TM Lead	Sonia Hammache	Sonia.Hammache@e.doe.gov

## Decarbonization Pillars and EERE Emphasis Areas

- CUBI acids will focus on the decarbonization pillar of low-carbon fuels by continuing to develop and sufficiently derisk pathways to convert waste products to sustainable aviation fuel in support of the DOE's 2030 and 2050 goals to replace 10% and 100% of domestic aviation fuel with sustainable alternatives by demonstrating new upgrading processes and exploring catalyst durability at laboratory scales. We will continue to support workforce development and diversity by supporting a Colorado School of Mines graduate student and summer interns on project work.

# CUBI (PNNL): Catalytic Upgrading of 2,3-Butanediol (BDO) to Fuels

## /WBS#2.3.1.102

Vanessa Dagle/PNNL

WBS# - 2.3.1.102

### Project Objectives

This task aims to support the overall CUBI effort for de-risking and optimizing catalytic processes to assist commercialization efforts by converting biologically-derived 2,3-BDO from a mixed sugar fermentation process into jet-range hydrocarbons with the ability to a) reach 70% GHG emissions reduction and b) obtain a distillate MFSP of \$2.50/GGE by 2030.

### Technical Approach

Development of the SOT pathway for conversion of aqueous 2,3-BDO to SAF via methyl ethyl ketone without vaporization of water to help reduce energy demand and GHG emissions. Investigate downstream olefins oligomerization and hydrogenation to help control the fuel properties and meet ASTM specifications for jet fuel blendstock.

### Project Milestones and Outcomes

- Starting at TRL 3 and projected ending at TRL 4-4.5
- **End of project milestone:** De-risk end-to-end 2,3 BDO intermediate upgrading processes to SAF to clearly articulate cases for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions targeting <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.
- **Go/No-Go:** Convert 2,3-BDO to SAF and demonstrate sustainable aviation fuel production blendstock through demonstration of each step and demonstrate that the blendstock candidate meets key ASTM specifications for jet fuel blendstock. Achieve 75% jet fuel range hydrocarbons fraction after oligomerization of the C<sub>4</sub>-C<sub>5</sub> rich olefins mixture and demonstrate ≤ 5% olefins in the final jet fuel blendstock. (09/30/2024)

### Decarbonization Pillars and EERE Emphasis Areas

- *Strategic goal: Decarbonize transportation sector- SAF production*
- *This task will focus its R&D effort to support the overall CUBI project for de-risking commercialization efforts related to SAF production from biologically-derived intermediates targeting BETO's 2040 goals of 17 MM gallons and its goal of 70% GHG emissions reduction.*
- *How: by demonstrating a cost-effective integrated process for conversion of aqueous 2,3-BDO to SAF, by upgrading 2,3-BDO to MEK intermediate without separation or vaporization of water from the feed to reduce energy demand and GHG emissions and by demonstrating control of the molecular structure of the downstream product from oligomerization and hydrogenation to target a jet blendstock meeting ASTM criteria.*

### Project Attributes

Project Start and End Dates	October 1, 2022- September 30, 2025	
FY23 Budget	Total: \$450K (PNNL)	
Collaborations	ACSC WBS 2.5.1.304, CDM WBS 2.5.4.501	<a href="mailto:Susan.habas@nrel.gov">Susan.habas@nrel.gov</a> , <a href="mailto:Huamin.wang@pnnl.gov">Huamin.wang@pnnl.gov</a>
DOE TM Lead	Sonia Hammache	<a href="mailto:Sonia.Hammache@ee.doe.gov">Sonia.Hammache@ee.doe.gov</a>

# Catalytic Upgrading of 2,3-BDO Intermediates (LANL)

Xiaokun Yang (Claire)/LANL

## Project Objectives

- In support of CUBI objectives, this work will focus on upgrading fermentation-derived into sustainable aviation fuel 2,3-BDO via dioxolane intermediates. Identifying new and improved catalyst compositions and reaction process for the integrated conversion of BDO fermentation broth with aldehyde to SAF, targeting at a distillate MFSP of \$2.50/GGE and GHG emissions reduction at 70%.

## Technical Approach

- Minimizing the broth impurities' effect on dioxolane formation and downstream upgrading to olefins/SAF with catalyst and reaction process development.
- Production of dioxolanes with BDO fermentation broth and aldehydes (e.g., acetaldehyde) in batch reaction and evaluate process in flow reaction systems.
- Delivering > 50mL of dioxolane products to ORNL for downstream upgrading

Project Type: Continuation

## Project Attributes

Project Start and End Dates	October 1, 2022- September 30, 2025	
FY23 Budget	\$250K (LANL)	
Collaborations	Andrew Sutton	suttonad@ornl.gov
DOE TM Lead	Sonia Hammache	<a href="mailto:sonia.hammache@ee.doe.gov">sonia.hammache@ee.doe.gov</a> 202-384-2183

WBS# - 2.3.1.103

## Project Milestones and Outcomes

- Starting TRL 3 and Ending TRL 4
- End of project goal/milestones: De-risk end-to-end biochemical intermediate upgrading processes to SAF to clearly articulate cases for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions targeting <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.
- Go/No-Go's w/date (FY24 Q4) Update and evaluate process improvements on LCA/TEA based on catalyst improvements, separations and process development to de-risk further development of this pathway. Go: Identify improvements that demonstrate potential for > 70% GHG reduction and cost of < \$2.50gge. No Go: PNNL, ORNL and LANL will work jointly to accelerate the commercial deployment of the preferred pathway for 2,3-BDO upgrading to sustainable aviation fuel.

## Decarbonization Pillars and EERE Emphasis Areas

*This project will continue R&D to address strategic goal in transportation (SAF) pillar such that subsequent commercial SAF production is de-risked targeting at BETO's goals of 17 MM gallons commercial SAF production and decarbonization by 2040, by activities: (1) developing new catalyst compositions for key intermediate (e.g., dioxolane) formation, enabling low-cost reactive separation process, (2) enabling the integration of ethanol fermentation process by producing dioxolane with 2,3-BDO and acetaldehyde, and (3) working as a team to demonstrate the ASTM qualified production of SAF and > 70% of GHG reduction.*

# Catalytic Upgrading of Biochemical Intermediates (CUBI) (ORNL)

Andrew Sutton (ORNL)

WBS# - 2.3.1.104

## Project Objectives

- In support of overall CUBI project objective, this task aims to convert biologically-derived 2,3-BDO from a mixed sugar fermentation process into jet-range hydrocarbons with the ability to obtain a distillate MFSP of \$2.50/GGE and reduce GHG emissions by at least 70%

## Technical Approach

- Develop technologies for converting fermentation-derived 2,3-BDO to middle distillates and coproducts via dioxolane intermediates. Fuel property analysis will be used to guide catalyst and process development.

Project Type: Ongoing AOP (core ChemCatBio project)

## Project Milestones and Outcomes

- Starting TRL 3 and Ending TRL 4
- End of project goal: De-risk biochemical intermediate upgrading processes to SAF to enable technology for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions of <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of a reasonable fuel MFSP (i.e., ~\$2.50/gge).
- Go/No-Go's w/date (18 months) : Achieve at least 80% carbon efficiency for single step oligomerization of produced olefins to SAF range hydrocarbons using an engineered catalyst. If unsuccessful evaluate the use of more complex and costly multi-step oligomerization technology.

## Project Attributes

Project Start and End Dates	October 1, 2022 – September 30, 2025	
FY23 Budget	Total: \$400k (ORNL)	
Collaborations	LANL: Claire Yang	<a href="mailto:xioakuny@lanl.gov">xioakuny@lanl.gov</a>
DOE TM Lead	Sonia Hammache	sonia.hammache@ee.doe.gov

## Decarbonization Pillars and EERE Emphasis Areas

- This project will address the BETO strategic SAF production challenge (3 billion gallons/year by 2030, total decarbonization of aviation by 2050) by demonstrating production of specification-compliant aviation fuels or blendstocks from renewable feedstocks via deployable catalytic processes.
- We will leverage our current industry collaborations and foster new ones as needed to address industry needs and enrich our analytical models to demonstrate potential for producing biofuel market competitive SAF with >70% GHG emissions reductions compared to petroleum derived fuels.
- The end-of-project goal is to demonstrate process integration for production of SAF meeting ASTM criteria under industrially relevant conditions to ensure a seamless transition from bench scale to pilot scale.

# CUBI (NREL): Catalytic Upgrading of Mixed Sugars Derived Furfurals

David K. Johnson

WBS# - 2.3.1.101

## Project Objectives

This task supports the overall CUBI effort to de-risk and optimize catalytic processes to assist commercialization efforts by converting furfurals in mixed sugar hydrolysates into jet-range hydrocarbons with the ability to a) reach 70% GHG emissions reduction and b) obtain a hydrocarbon product with a MFSP of \$2.50/GGE by 2030 .

## Technical Approach

Modify the current pathway to produce C10-C12 bicyclic alkanes instead of n- and iso- alkanes. The bicyclic alkane product will have SAF-advantaged properties, fitting into the center of the jet boiling range and featuring higher energy density than n-alkanes (39.5 MJ/L vs 34.8 MJ/L for n-decane). Sugars in biomass hydrolysates will be converted to furfurals and then converted to a mixture of cyclopentanones by catalytic HDO under mild conditions (140-160 °C, 30-40 bar H<sub>2</sub>).

**Project Type:** on-going AOP (new cycle)

## Project Milestones and Outcomes

- Starting at TRL 3 and projected ending at TRL 4
- **End of project milestone:** De-risk end-to-end furfurals upgrading processes to SAF to clearly articulate cases for industrial adoption through mitigation of scalability roadblocks, measurement of finished fuel properties and quantification of blend limitations, demonstration of life-cycle GHG emissions targeting <27 g CO<sub>2</sub>eq/MJ (70% reduction relative to fossil jet), and calculation of MFSP targeting \$2.50/GGE.
- **Go/No-Go:** Evaluate new pathway through furfurals-derived cyclopentanone intermediates to produce a high energy density bicyclic alkane SAF blendstock. In the critical step of furfurals-to-cyclopentanones, achieve a 50% carbon-yield using a biomass hydrolysate-derived furfurals mixture. (09/30/2024)

## Decarbonization Pillars and EERE Emphasis Areas

- Strategic goal: Decarbonize transportation sector- SAF production
- This task will focus its R&D effort to support the overall CUBI project for de-risking commercialization efforts related to SAF production from biologically-derived intermediates targeting BETO's 2040 goals of 17 MM gallons and its goal of 70% GHG emissions reduction.
- How: by demonstrating a cost-effective integrated process for converting mixed sugars in biomass hydrolysates initially into furfurals and then into a mixture of cyclopentanones by catalytic hydrodeoxygenation (HDO). Self-condensation of the cyclopentanones followed by HDO will yield bicyclic alkanes that have excellent properties for blending into a jet fuel that meets ASTM criteria.

## Project Attributes

<b>Project Start and End Dates</b>	October 1, 2022- September 30, 2025	
<b>FY23 Budget</b>	Total: \$854K (NREL)	
<b>Collaborations</b>	ACSC 2.5.1.304, CCPC 2.5.1.302	<a href="mailto:Susan.habas@nrel.gov">Susan.habas@nrel.gov</a>
<b>DOE TM Lead</b>	Sonia Hammache	Sonia.Hammache@ee.doe.gov



# Response to Select Reviewer Comments

*...the true value to BETO may be to keep the biomass sugar-derived 2,3-BDO as a solvent for new uses, in my opinion, to reduce the final cost of other routes to fuel.*

We appreciate the recognition of the recent progress made within this project. While we are aware of 1,4-BDO use as solvent, we have not found industrial application as a solvent for 2,3-BDO. We found that it is typically converted into MEK, which is itself used as solvent. The global 1,2-propanediol market is equal to 2.7 million tons/year (2020). It is not a large market, and, as such, if 2,3-BDO were to replace 1,2-propanediol as a solvent, an excess of 2,3-BDO would still be available. This excess 2,3-BDO could be used for fuels and chemicals production. Catalytic upgrading of 2,3-BDO to solvents or other products and fuels can help to expand its market application.



# Response to Select Reviewer Comments

*...the CUBI project is expansive, and research thrusts therein are, at times, not directly connected (e.g., BDO upgrading and furan pathways are essentially independent). The specific leadership structure and management hierarchy were somewhat unclear, so I could not really determine if each lab runs independently pursuant to specific goals there or if there is a central point of contact (POC) responsible for coordinating research across the four labs.*

We appreciate the comment regarding the wide breadth of activities being conducted within the CUBI project. There are many advantages for all of the catalytic upgrading efforts within the broader biochemical conversion pathways to be performed within a single coordinated effort that spans work at several national labs, which was the approach recommended approximately 6 years ago—before which these efforts were conducted as individual projects in a less coordinated manner. The current management structure involves a central coordination effort at NREL, where much of the associated process development and TEA support for the overall biochemical conversion pathway is conducted. We made an effort to explain this structure in more detail in the FY23 presentation.





# Response to Select Reviewer Comments

*...Regarding numerous comments surrounding co-products and cost reductions:*

Coproduct opportunities have been emphasized in a greater manner in this project during the last 2 years to lessen the exclusive dependence on lignin-derived coproducts in biochemical conversion pathways to enable fuel cost targets. Additionally, utilizing corn starch-derived hexose sugars in existing corn ethanol commercial plants can provide a near-term opportunity to repurpose such facilities away from ethanol production to produce higher-value product revenue streams using existing commercial-scale fermentation capacity.

## **Publications, Patents, Presentations, Awards, and Commercialization**

- **List any publications, patents, awards, and presentations that have resulted from work on this project**
- **Use at least 12 point font**
- **Describe the status of any technology transfer or commercialization efforts**


Note: This slide is for the use of the Peer Reviewers only – it is not to be presented as part of your oral presentation. These Additional Slides will be included in the copy of your presentation that will be made available to the Reviewers.

# Furans Pathway: Path Forward

- Published a “mini-design report” for this pathway (2021)
- Future 2030 target case identified similar overall MFSP potential as biological pathways
  - Substantially higher fuel yields (61+ GGE/ton vs 43-45 GGE/ton)
  - Offset by higher OPEX costs, primarily hydrogen and NG (LCA drivers)
- Latest 2022 improvements would reduce 2030 target MFSPs by ~\$0.20/GGE (dedicated or integrated case)
  - Also nearly 50% reduction in NG usage – very promising, but LCA still needed to compare against biological design cases

	Dedicated Biorefinery	Integrated Biorefinery
Feedstock rate	2,205 dry U.S. tons/day	
Online time	7,884 h/yr (90% online factor)	
Total fuel yield	108.4 GGE/dry U.S. ton feedstock	61.2 GGE/dry U.S. ton feedstock
Total fuel production rate	78.5 MM GGE/yr	44.3 MM GGE/yr
Adipic acid coproduct yield	284 lb/dry U.S. ton feedstock	276 lb/dry U.S. ton feedstock
Adipic acid production rate	205 MM lb/yr	200 MM lb/yr
Total variable OPEX excluding coproducts	\$269 MM/yr	\$187 MM/yr
Coproduct revenue	\$193 MM/yr	\$188 MM/yr
Total fixed OPEX	\$20 MM/yr	\$20 MM/yr
Total equipment cost	\$414 MM	\$416 MM
Total capital investment	\$787 MM	\$786 MM
TCI per annual gallon	\$10.02/GGE	\$17.75/GGE
<b>Minimum Fuel Selling Price</b>	<b>\$2.54/GGE</b>	<b>\$2.72/GGE</b>
Feedstock contribution	\$0.66/GGE	\$1.17/GGE
Fuel conversion contribution	\$3.11/GGE	\$3.71/GGE
Coproduct conversion contribution	-\$1.23/GGE	-\$2.16/GGE

Further  
\$0.20/GGE  
savings per  
2022 updates



**Techno-Economic Assessment for the Production of Hydrocarbon Fuels via Catalytic Upgrading of Furans**

Bruno Klein, Ian McNamara, Ryan Davis, Ashutosh Mittal, and David Johnson

*National Renewable Energy Laboratory*

NREL is a national laboratory of the U.S. Department of Energy  
Office of Energy Efficiency & Renewable Energy  
Operated by the Alliance for Sustainable Energy, LLC

Technical Report  
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September 2021

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