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DOE Bioenergy Technologies Office (BETO) 2015 Project Peer Review

Characterization and Valorization of Aqueous Phases Derived from Liquefaction and Upgrading of Bio-oils WBS: 2.3.1.310

March 27, 2015

Thermochemical Conversion Technology Area Review

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Pacific Northwest National Laboratory

PNNL-SA-108318

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Challenge: Direct liquefaction processes produce aqueous streams

1. The streams are poorly understood
2. The streams contain expensive feedstock carbon in the form of low molecular weight oxygenates

Solution: Fill the aqueous phase knowledge gap and develop processes to maximize the value of the aqueous phase carbon

1. Characterize a wide variety of aqueous streams for all bioenergy stakeholders
2. Develop processes to produce chemicals, H₂, and/or additional fuel from aqueous phase organics

▶ Tangible benefits to the United States: Reduce technical and economic risks associated with bioeconomy implementation leading to American jobs and lessened dependence on foreign fossil resources

Quad Chart Overview

Timeline

- ▶ Project start date: Oct. 1, 2013
- ▶ Project end date: Sept. 30, 2017
- ▶ Percent complete: 38%

Budget

	Total Costs FY 10 – FY 12	FY 13 Costs	FY 14 Costs	Total Planned Funding (FY 15- Project End Date)
DOE Funded	0	0	\$1.33 MM	\$5.27 MM
Project Cost Share (Comp.)	0			

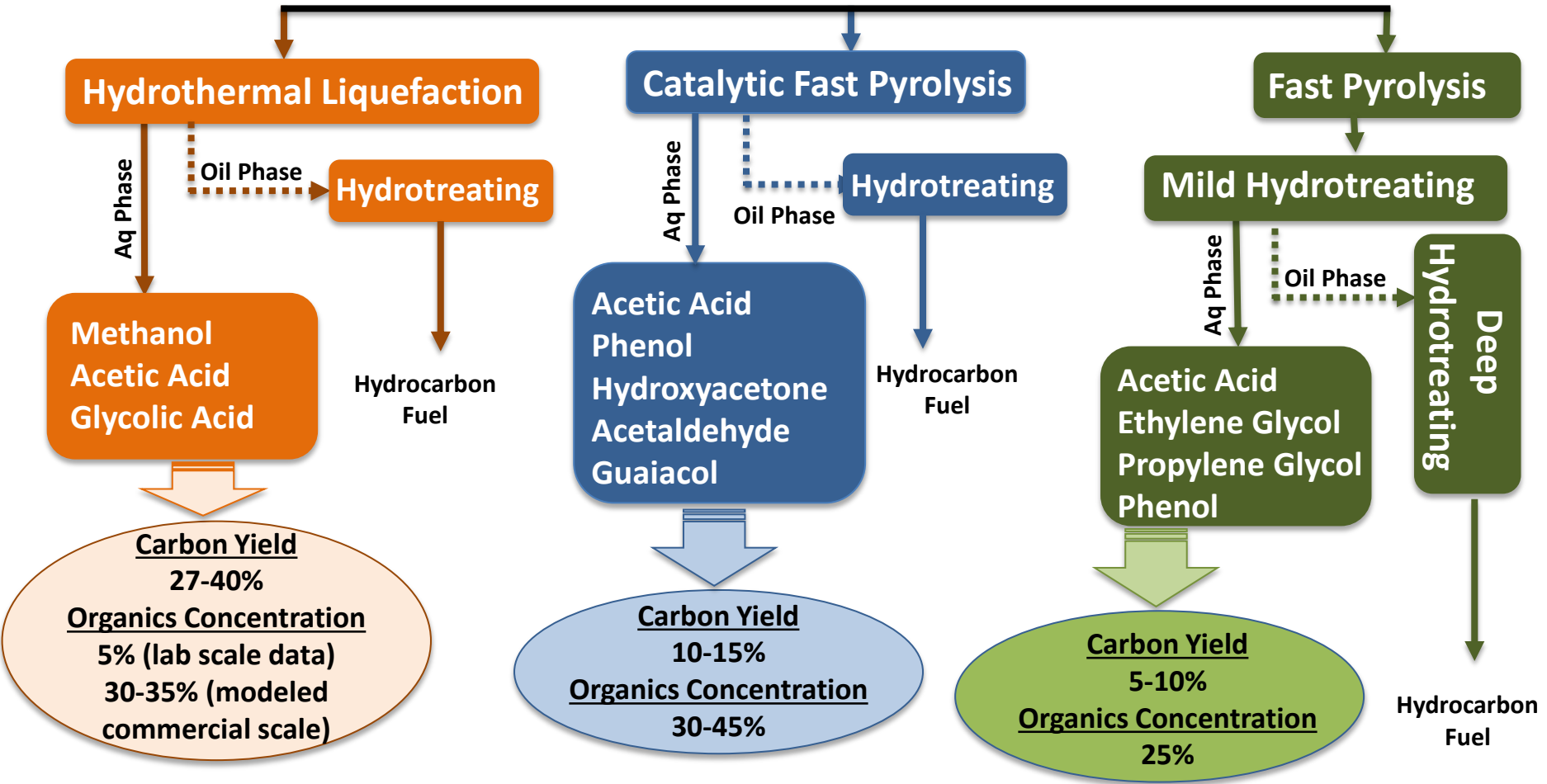
Barriers

- ▶ Barriers addressed
 - Tt-N. Aqueous Phase Utilization and Wastewater Treatment
 - Tt-M. Hydrogen Production
 - Tt-L. Knowledge Gaps in Chemical Processes

Partners

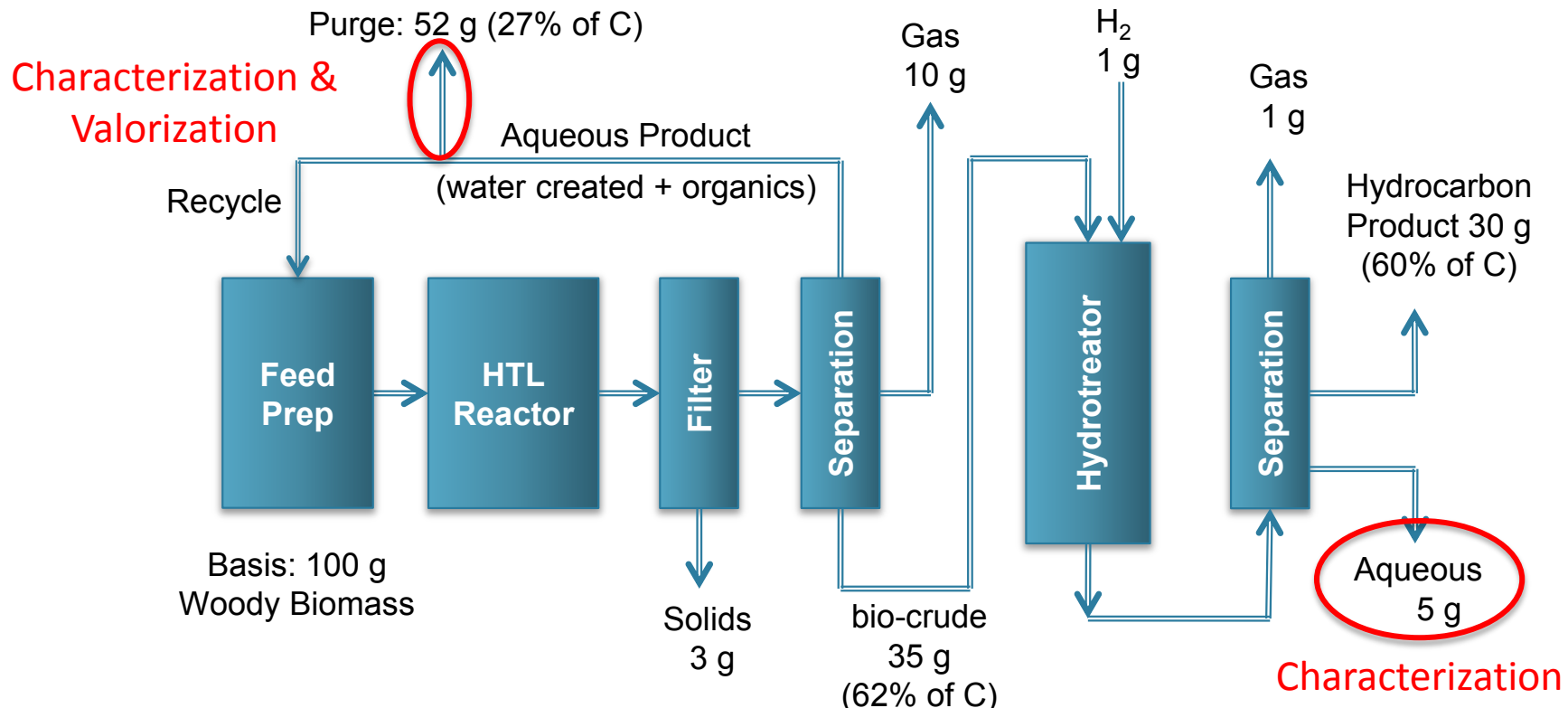
- Aqueous samples from partners
 - Genifuel, Inc.
 - NREL
 - VTT
 - Feedstock interface (2.2.1.305)
 - Hydrothermal Processing of Biomass (2.2.2.301, 2.4.1.303)
 - Core R&D for Pyrolysis to Fuels (2.3.1.302)
 - Thermochemical Interface (1.3.4.101)
 - Whole Algae Liquefaction Model Development (1.3.4.100)
 - Production and Upgrading of Infrastructure Compatible Bio-Oil with VTT (2.11.2.11 – FY 14 WBS)

1 - Project Overview



1 - Project Overview

- ▶ Characterizing aqueous streams benefits all bioenergy stake holders
- ▶ Valorizing aqueous phase C will significantly improve process economics
 - **Increase Credits:** Add valuable co-products (chemicals, hydrogen, more fuel)
 - **Decrease Expenses:** Lower or eliminate natural gas; lower wastewater volume



Currently: “**Poorly understood aqueous waste streams**”

Project Goal: “**Well defined aqueous feedstocks**”

2 – Approach (Technical)

- ▶ Three tasks simultaneously investigating aqueous streams
 1. Characterization – Produce robust datasets and disseminate data to the benefit of all bioenergy stakeholders
 2. Catalytic Conversion – producing chemicals to add value *in concert* with fuels, not in place of them
 3. Steam Reforming – producing H₂ to decrease or eliminate required external natural gas and lower GHG emissions
- ▶ General approach
 - Employ rigorous analytical chemistry methods to produce robust data sets
 - Catalytic process development using flow reactors
 - Emphasis on testing real biomass-generated aqueous streams
 - Techno-economic analysis (TEA) modeling to guide research and measure economic impact of developing processes
- ▶ Primary metrics
 - Overall process fuel production costs – Go/No Go metric
 - Conversion, selectivity, catalyst stability
 - GHG reduction

2 – Approach (Management)

- ▶ Project Management Plan Implemented
 - ☑ Merit Reviewed AOP – July 2014 – Generally positive comments and excellent suggestions to help guide further research
 - ☑ Quarterly internal milestones – Currently all met and on track to continue
 - ☑ Annual deliverables -- Characterization manuscripts in September each year
 - ☐ Annual major milestones – TEAs to gauge the effect of the developing technologies on MFSP on apples-to-apples basis vs. anaerobic digestion
 - ☐ Go/No Go – February 2016: *“Demonstrate a 5% reduction in the cost of fuel processing vs. aqueous phase anaerobic digestion...”*
- ▶ Critical Success Factors
 1. Developed processes must add economic benefit (i.e. improve the bottom line)
 2. Catalysts and processes must be able to stably withstand aqueous environments
- ▶ Challenges
 1. Catalyst stability in aqueous environments – a challenge across the bioenergy space and an opportunity for widespread interactions
 2. Potentially aggressive (e.g. acidic) feed streams with dissolved inorganics



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Characterization

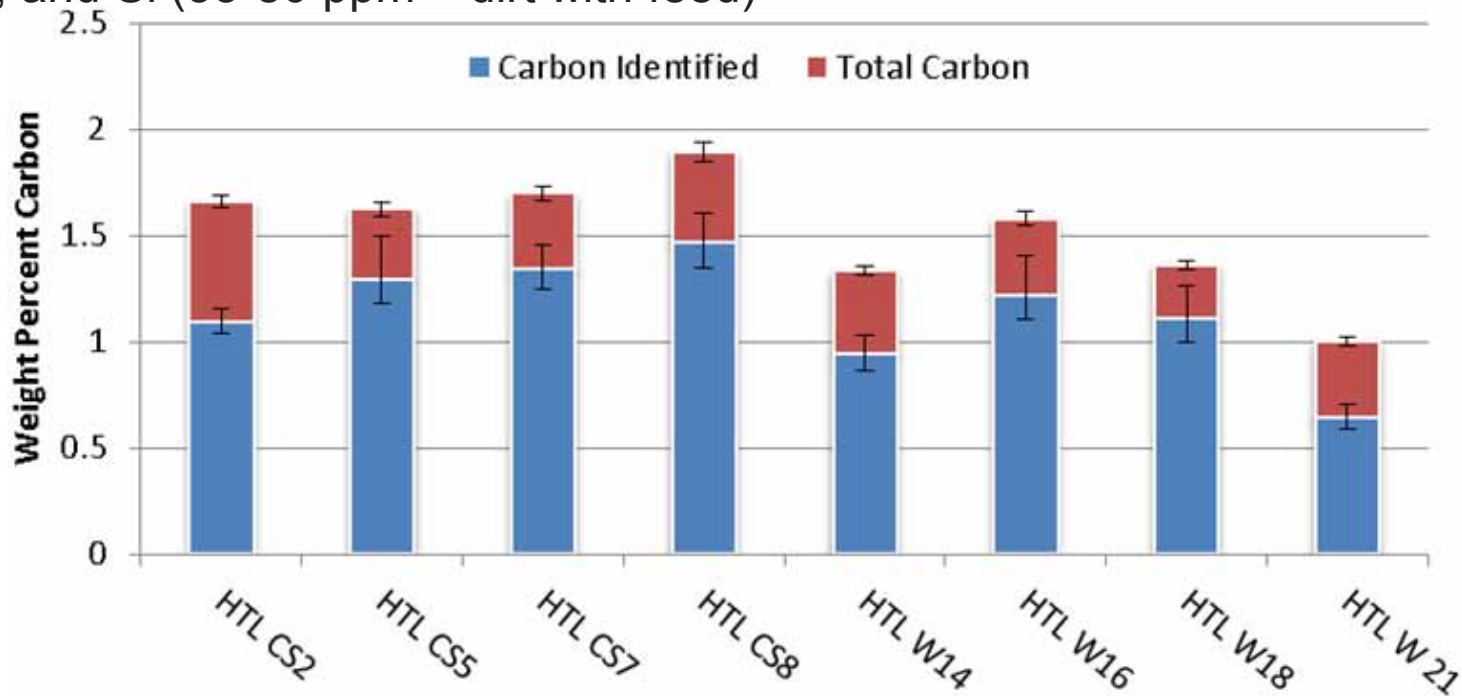
3 – Technical Accomplishments/ Progress/Results – Characterization

- ▶ Very little data regarding aqueous streams is available – and a lot of that is qualitative (e.g. MS area counts)
- ▶ Rigorous quantitative analysis of aqueous streams addresses knowledge gap
 - Quantification using acquired standards
 - Quadruplicate tests, randomized block design according to NIST standards
 - HPLC, GC-MS, GC-FID, TC, ICP-OES, COD, IC (anions and cations)
- ▶ Total carbon (TC) identifies all carbon in the aqueous sample
- ▶ TC compared with amount quantified using standards
- ▶ High priority aqueous samples
 - Hydrotreating of fast pyrolysis oil
 - Hydrothermal liquefaction of terrestrial feedstocks
 - Hydrothermal liquefaction of aquatic feedstocks
 - Catalytic fast pyrolysis
- ▶ Data disseminated via peer reviewed manuscripts and presentations to the benefit of all bioenergy stakeholders

3 – Technical Accomplishments/ Progress/Results – Characterization

Bench Scale HTL Aqueous Phase

- ▶ Quantified Carbon – Primarily low molecular weight oxygenates
 - Acids (~70% of C, glycolic, acetic, formic, propanoic)
 - Alcohols (~20% of C, methanol, ethanol, propanol, glycols)
 - Ketones (~8% of C, acetone, cyclopenta-ones)
 - Phenolics (~2% of C, phenol, methoxyphenol, ethylphenol)
- ▶ Primary inorganics: Na (~2000-7000 ppm – NaCO₃ buffer), K (120-1400 ppm – from feed), and Si (35-80 ppm – dirt with feed)





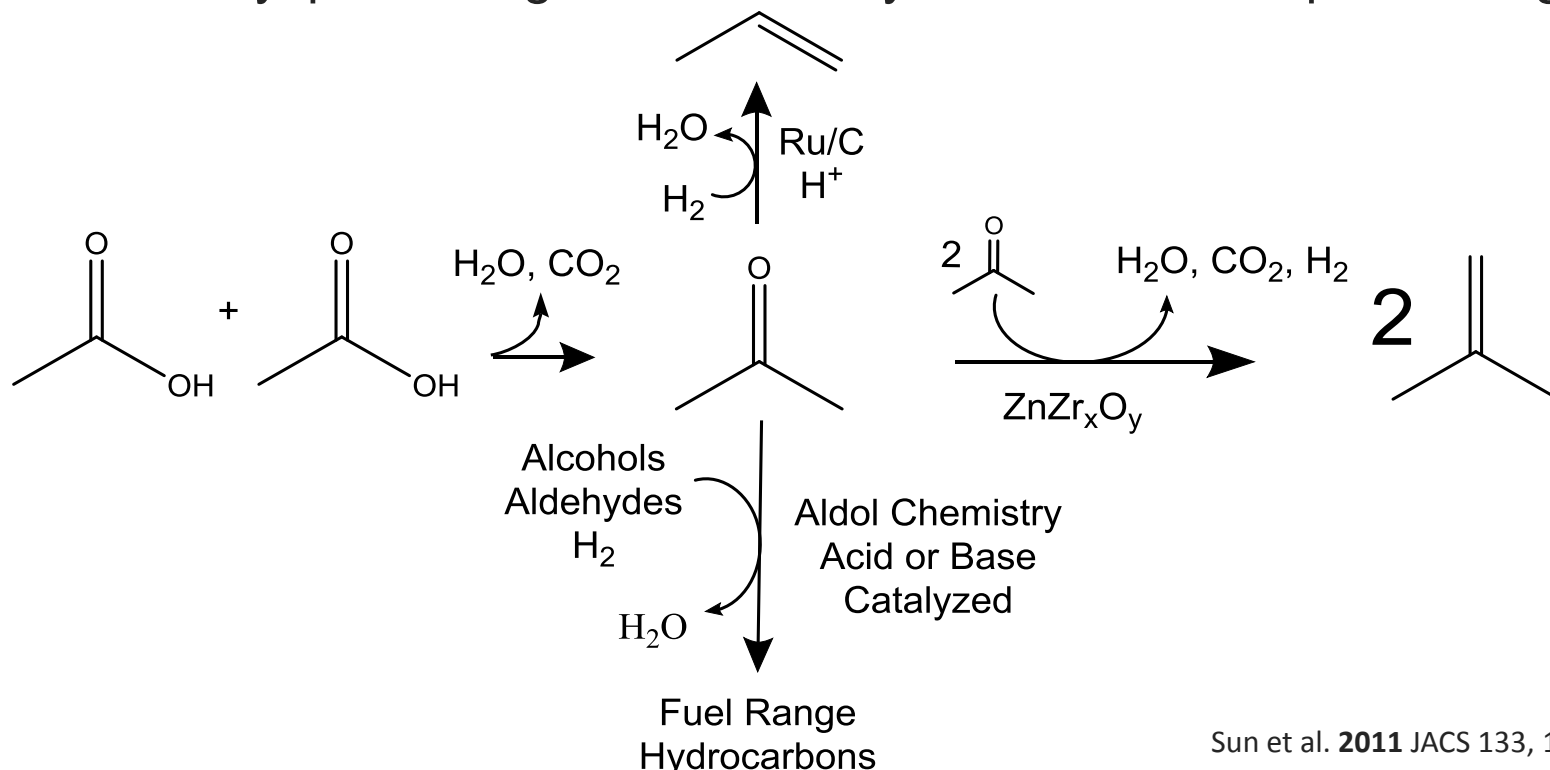
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Catalytic Conversion

3 – Technical Accomplishments/ Progress/Results – Catalytic Conversion

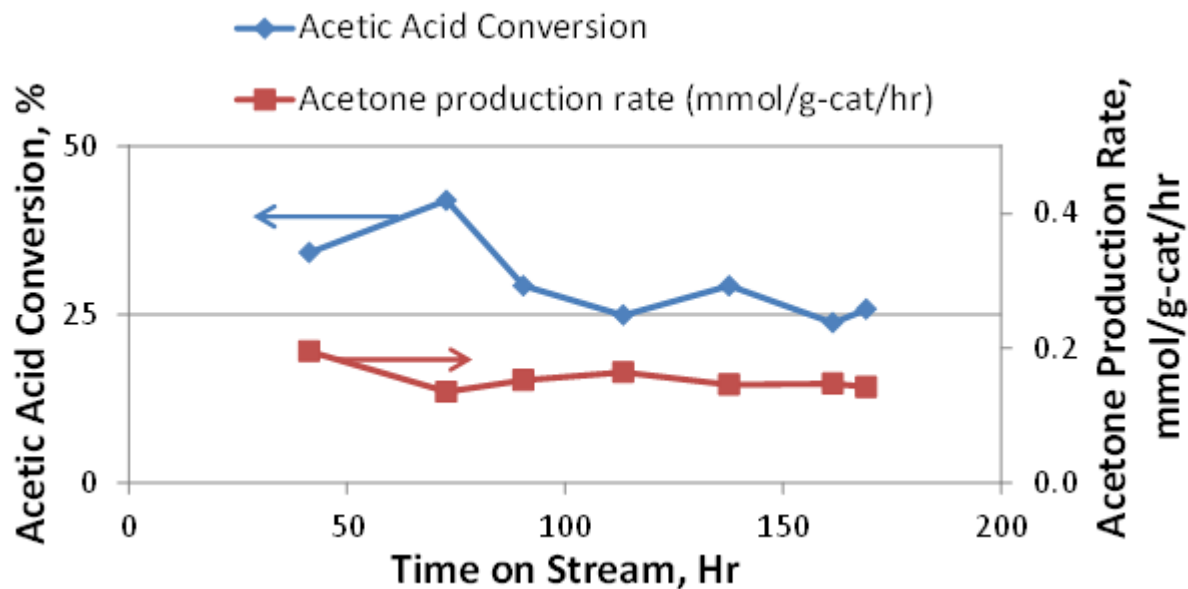
- ▶ Ubiquitous organic acids are a challenge in aqueous streams
 - Low volatility – water distills from acids (not the other way around)
 - Limited downstream processing options
- ▶ Covert C_2+ acids via ketonization to ketones
 - Eliminates oxygen with no H_2 required
 - Carbonyl provides greater flexibility for downstream processing options



3 – Technical Accomplishments/ Progress/Results – Catalytic Conversion

More than 25 ketonization catalysts screened to date

Promising catalysts identified via screening tested in upflow fixed-bed reactor



Biomass-Derived HTL Aqueous Feed LC Data (wt%)	
Acetic Acid	22.5
Propanoic Acid	4.1
Methanol	2.7
Glycolic Acid	1.8
Propylene Glycol	0.9
Ethanol	0.5
Butanol	0.3
Ethylene Glycol	0.1
Others	0.1

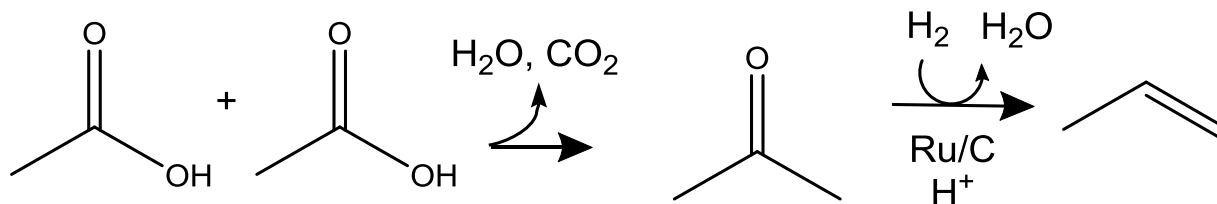
ICP Data (ppm)	
Na	4703
K	171
Ca	71
Si	25
Mg	13
Mn	9

- $\text{La}_2\text{O}_3/\text{ZrO}_2$, 300°C, 1350-1400 psig, WHSV = 0.37 hr⁻¹
- Most active catalyst to date (shown above) is stable for > 150 hr with biomass-derived feed
- Activity lower with “real” feeds – investigations underway

Production of propylene and butylene from mildly hydrotreated fast pyrolysis aqueous phase also demonstrated via ketonization/reduction/dehydration route

3 – Technical Accomplishments/ Progress/Results – Catalytic Conversion

- ▶ HTL of lignocellulosic feedstock to fuel model – preliminary results
- ▶ Aqueous phase options: Baseline (anaerobic digestion) vs. catalytic conversion to olefins
 - Ketonization/reduction/dehydration to propylene & butylene



Example of chemistry to convert organic acids into olefins

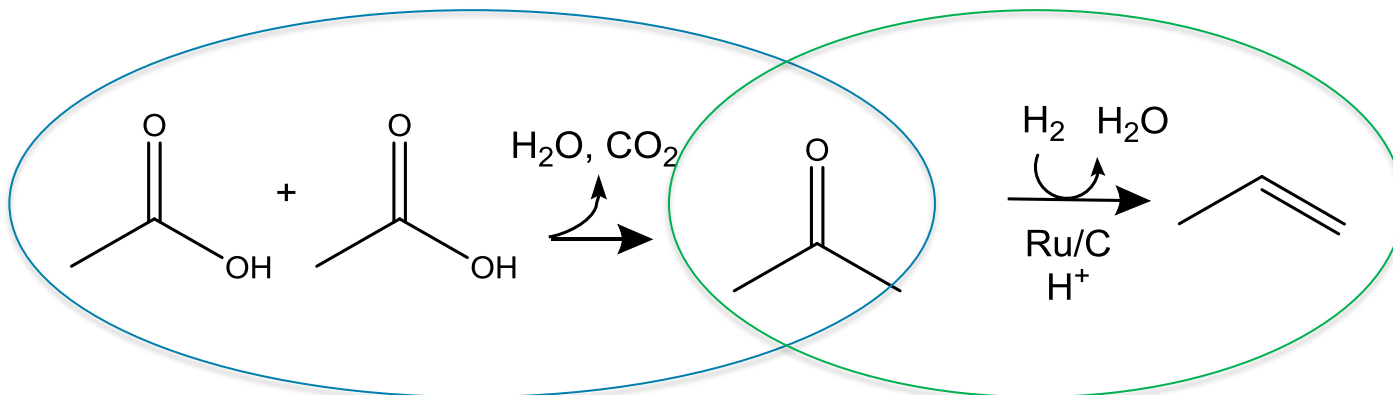
- Model based on ketonization data acquired with biomass-derived feed
- Capital costs increased ~45% – of which ~85% due ketonization process
- Operating costs increased ~15%

Bottom Line when Olefin Credits Added*

Aggregate fuel production cost:
Anaerobic digestion: \$3.25/gal
Catalytic conversion to olefins: \$2.08/gal
Increase ketonization WHSV 5x: \$1.51/gal

3 – Technical Accomplishments/ Progress/Results – Catalytic Conversion

- ▶ Techno-economic modeling is helping us focus our research
 - Condensed phase ketonization processing
 - Avoids energy intensive vaporization of water-rich stream
 - Allows direct processing high ash feed
 - Ketonization product can be distilled economically from water
 - Capital increase in TEA model demonstrates need for greater ketonization kinetics



Capital intensive process
Cutting-edge research in
process & catalyst development

Relatively inexpensive process portion
Well understood chemistry
Commercially practiced

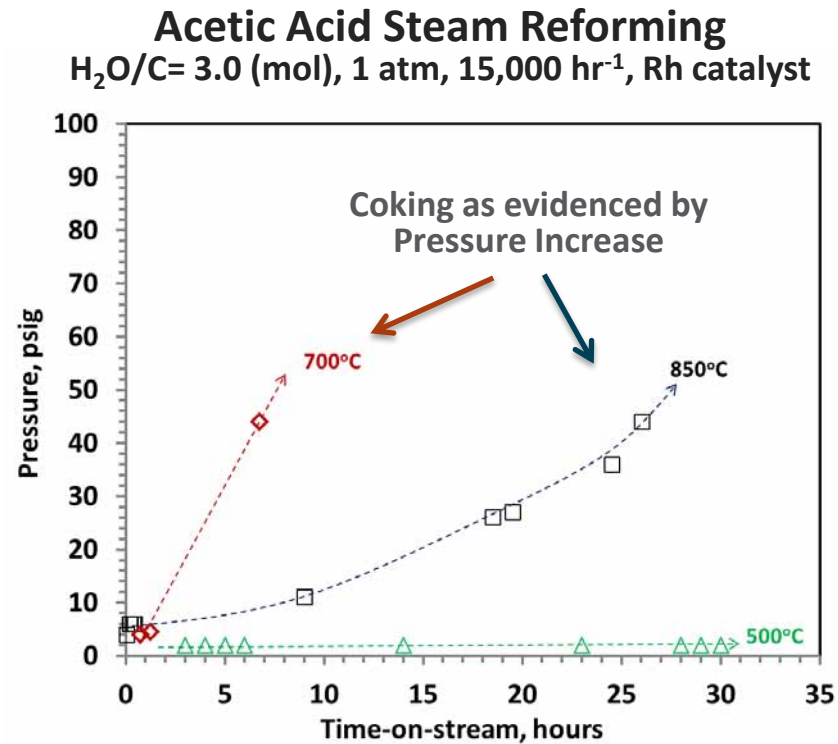
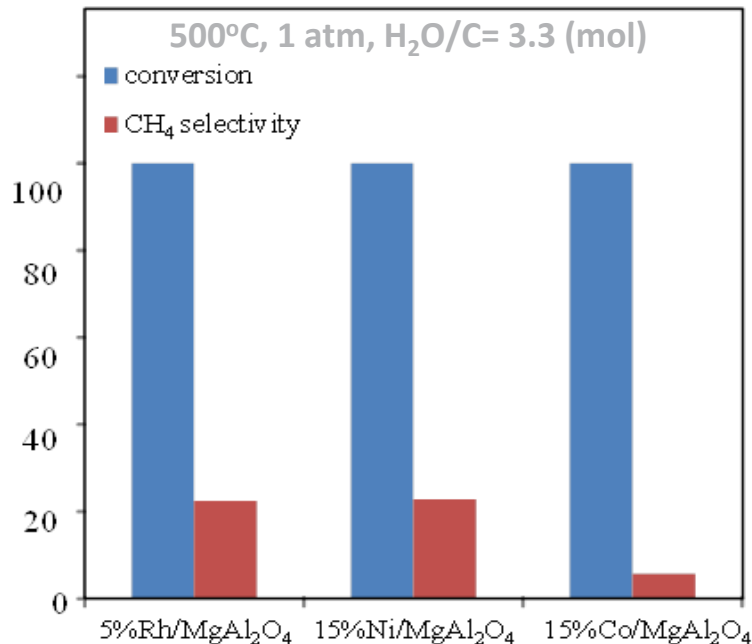


Steam Reforming

3 – Technical Accomplishments/ Progress/Results

Steam Reforming – Process Development

- ▶ Operating > 550°C leads to severe coking
- ▶ Operating at 500°C gives stable performance
- ▶ Petroleum analogy: A two-step process for steam reforming naphtha
 1. **Pre-reformer:** ~500°C operation prevents catalyst coking
 2. **Methane steam reformer:**
 - 600-850°C operation maximizes H₂
 - Already included in biorefinery designs



- ▶ Cobalt (Co) is **less selective** towards methane than more conventional Ni and Rh steam reforming catalysts

3 – Technical Accomplishments/ Progress/Results

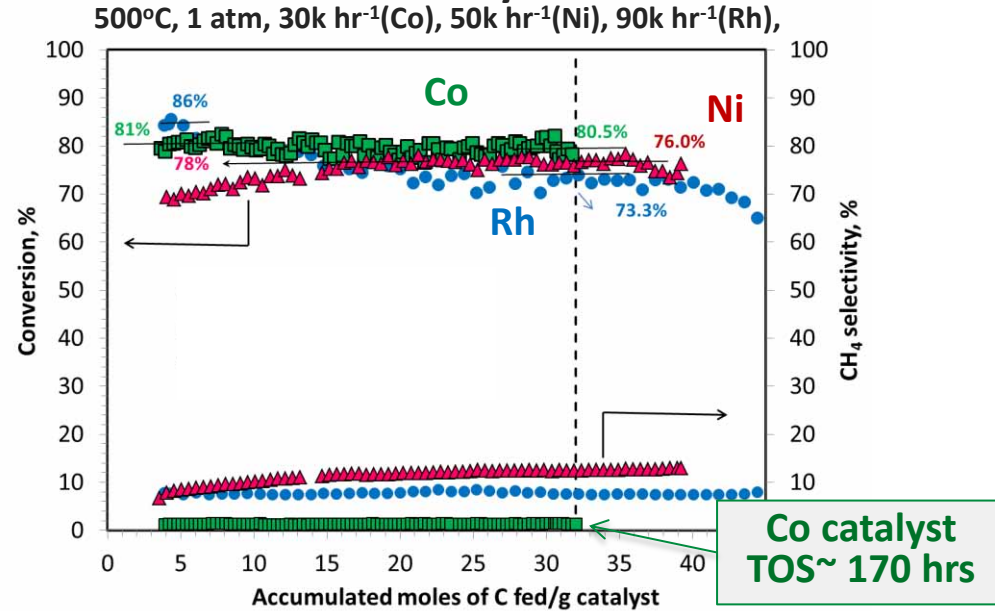
Steam Reforming – Catalyst Development

Model Feed (mild-HT FP)

Chemical name	Formula	Composition, wt%
Acetic acid	C ₂ H ₄ O ₂	6.3
Phenol	C ₆ H ₆ O	6.0
Ethylene glycol	C ₂ H ₆ O ₂	4.9
Propylene glycol	C ₃ H ₈ O ₂	4.7
Tetrahydrofuran alcohol	C ₅ H ₁₀ O ₂	1.3
1,4-butanediol	C ₄ H ₁₀ O ₂	1.3
Γ-butyrolactone	C ₄ H ₆ O ₂	1.3
Formic acid	CH ₂ O ₂	0.9
Water	H ₂ O	73

$H_2O/C = 3.5$ (mol)

Stability



- ▶ Steam reforming of oxygenated organic mixtures is feasible
- ▶ Co exhibits **very low selectivity** towards **methane** compared to Ni and Rh
- ▶ Co is also more **stable** over duration of tests conducted to date
- ▶ However, filamentous carbon formation observed via hrTEM is problematic for extended run durations
 - Currently developing a Co catalyst with enhanced resistance to carbon formation
 - Theoretical insights from computational chemistry are assisting with catalyst design

3 – Technical Accomplishments/ Progress/Results

Steam Reforming – Real Feed Evaluations

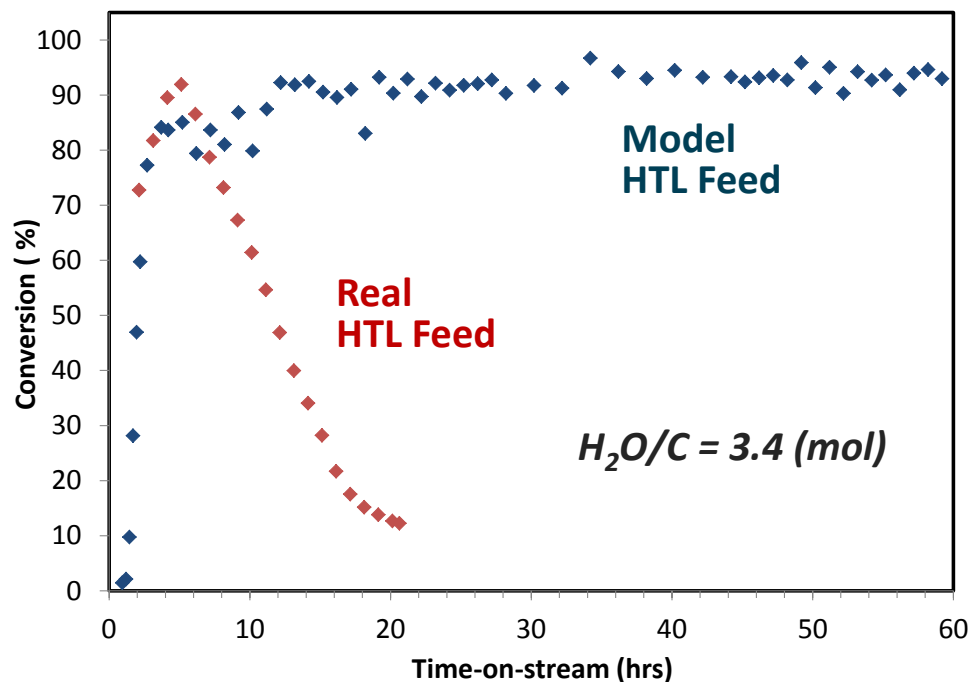


HTL—Derived Wood Feedstock (Wood-23)*

(wt.%)	Real HTL	Model HTL
Glycolic Acid	2.0	2.0
Acetic Acid	22.7	23.0
Ethylene Glycol	1.0	1.0
Propanoic Acid	4.2	3.8
Methanol	2.5	2.3
Ethanol	0.5	0.5
Butanol	0.3	0.2
Na (ppm)	6650	0
Mg (ppm)	28	0
K (ppm)	252	0
Ca (ppm)	135	0
S (ppm)	9	0

*additional organics were added to simulate HTL products with steady-state recycle

Steam Reforming over Co-based Catalyst 500°C, 1 atm, 15,000 hr⁻¹



- ▶ Steam reforming the oxygenates of an HTL feedstock is feasible
- ▶ However, inorganic contaminants (e.g., salts, sulfur) cause catalytic deactivation
- ▶ Deactivation observed with numerous biomass-derived samples
- ▶ Separation techniques are currently under evaluation (e.g., partial stream evaporation, ion exchange, liquid-liquid extraction, steam stripping, etc.)

4 – Relevance

- ▶ Direct liquefaction biorefineries will produce aqueous phases
- ▶ Aqueous phase characterization is imperative to proper design
 - All aqueous phases must be understood (regardless of value-added process opportunities)
 - Characterization/understanding beneficial to all stakeholders
- ▶ Maximizing the value of aqueous phase biogenic carbon will improve biorefinery commercial viability
 - Reduced economic risk
 - Additional product credits (chemicals, H₂, additional fuel)
 - Reduced debits (less or no natural gas, less wastewater)
 - Reduced technical risk – allows operators processing options

November 2014 MYPP Tt-N. Aqueous Phase Utilization and Wastewater Treatment:


“Research is needed to characterize organics in the aqueous phase and to convert these organics to hydrogen, biochemicals, or hydrocarbon fuels.” (emphasis added)

5 – Future Work

1. Characterize highest priority aqueous streams – algae HTL & lignocellulosic catalytic fast pyrolysis
2. Focus valorization processes development on real feeds and associated challenges
3. Utilize TEA modeling to guide research and determine economic benefits of valorization processes vs. anaerobic digestion

ML, DL, GNG	Description	15 Q3	15 Q4	16 Q1	16 Q2	16 Q3	16 Q4
ML	Establish baseline acetone production rates with 3 catalysts (Catalytic Conversion).						
DL	Submit a manuscript with aquatic biomass HTL aqueous phase data (Characterization)						
ML	Define the magnitude of the value for BETO in \$/gal vs. the baseline case of anaerobic digestion for a woody biomass HTL direct liquefaction process (Catalytic Conversion and Steam Reforming)						

5 – Future Work -- Continued

ML, DL, GNG	Description	15 Q3	15 Q4	16 Q1	16 Q2	16 Q3	16 Q4
ML	Identify and obtain FY16 high priority aqueous streams (e.g. municipal waste HTL, catalytic HTL, and/or mildly hydrotreated FP) to begin characterization and quantification of these streams (Characterization)						
Go/No Go	Demonstrate a 5% reduction in fuel processing cost is possible vs. anaerobic digestion for a direct liquefaction process through TEA modeling of the catalytic conversion and/or steam reforming processes using the best results obtained or through reasonable technological advancement (Catalytic Conversion and Steam Reforming)				 Go/No Go 2/29/2016		
ML	Determine the activity and stability for the catalysts utilizing a CFP-derived aqueous phase (Catalytic Conversion and Steam Reforming)						
ML	Determine the activity and stability for the catalysts utilizing aquatic-derived HTL aqueous phase (Catalytic Conversion and Steam Reforming)						
DL	Submit a manuscript to a peer reviewed journal detailing the results of aqueous phase characterization on the high priority streams identified through the Q1FY16 milestone. (Characterization)						

Summary

1. Aqueous phases will be produced by biomass direct liquefaction biorefineries
2. The characterization activity is facilitating understanding of the aqueous phases that is imperative for biorefinery design
3. We are also developing aqueous phase processing options to maximize the value of all biogenic carbon
4. PNNL is well positioned to access and acquire numerous aqueous streams through in-house capabilities (e.g. bench-scale HTL & hydrotreaters) and numerous collaborator contacts

We are reducing the technical and economic risks associated with biorefineries through aqueous phase characterization and biogenic carbon valorization

Acknowledgments

DOE Bioenergy Technologies Office

- Yunhua Zhu
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- Kurt Spies
- Heather Job
- Rich Hallen
- Andy Schmidt
- Rong Xing



Additional Slides

Responses to Previous Reviewers' Comments

2013 Peer Review Comments and Responses

1. **Comment:** “Move to “real” aqueous wastes as soon as possible. It would also be nice if samples of catalytic pyrolysis aqueous organics from NREL (and/or others) could be tested.”
 - **Response:** We’ve obtained real samples for characterization from external collaborators such as VTT and NREL. We plan to publish the results of the characterization from the VTT aqueous phase later this year. We have also tested several “real” aqueous phases in the upgrading and reforming processes produced from biomass at PNNL.
2. **Comment:** “Understanding fundamentals of C and H recovery and optimizing Aq phase recovery and utilization could be key to improving economics and efficiencies. Rebuilding a gasification pilot plant to study pyrolysis appears to be repurposing a pilot plant for which there was no longer any purpose to justify it's continued operations”
 - **Response:** Our original work plan involved producing specialized aqueous streams from fast pyrolysis (especially fast pyrolysis at higher temperature) for characterization. We have since re-scoped the characterization task to focus on the highest priority aqueous streams which are of primary interest to the bioenergy community today (e.g. HTL aqueous phases from terrestrial and aquatic biomass; CFP aqueous phases; hydrotreater water)

Responses to Previous Reviewers' Comments

► 2014 Merit Review AOP Comments and Responses

- 1. Comment:** “Although the characterization effort appears strong and should be valuable, it looks like the applicants may be missing the potential value of PROCESS characterizations (vs. analytical chemistry). Examples might include extractability in a number of organic solvents, “steam-strippability,” variation in overall solubility with temperature, acid/base characteristics of the aqueous solutes, and so on....might lead to a “partial vaporization” scheme wherein a (volatile) portion of the aqueous stream goes on to catalytic upgrading, while another (non-volatile) portion is best treated by, for example, anaerobic digestion.”

 - Response:** The comments received the AOP Merit Reviewers were very helpful. We have incorporated several of the received comments into our current laboratory investigations. For example, we’ve begun an experimental campaign investigating the partial vaporization of aqueous streams to determine the level of organics volatilized. We are also investigating steam stripping as an option; Aspen modeling using concentrations determined from biomass-derived aqueous phases are being used to inform the models and laboratory validation testing is planned.
- 2. Comment:** “Economically, hydrogen from steam-reforming of aqueous streams will need to compete with very inexpensive natural gas in many situations. If combined with substantial reductions in waste-treatment costs, it may still win out, but it also may be a break-even or worse.”

 - Response:** The point of the reviewer that steam-reforming of the organic aqueous phase compounds will compete with currently cheap natural gas is very well taken. However, as a commodity, the price of natural gas can be highly variable. Having a relatively stable and internally sourced supply of carbon available for steam reforming may be beneficial, especially if natural gas prices unexpectedly increase. By making TEA modeling an integrated focus of our research, we are able to determine the economic benefits of steam reforming and the interplay with savings realized from lower wastewater treatment costs. Indeed, we have included the economic effects within our progress metrics and management plan as annual milestones for various processes. It should be noted that most models for producing fuels from biomass include a H₂ plant (and thus, a reformer) already in the design. Additionally, lower GHG emissions are almost certain to be realized by reducing or eliminated externally required natural gas. Finally, it is possible that some aqueous streams will not be suitable for anaerobic digestion due to the presence of toxic compounds (e.g. phenol). In such a situation, steam reforming the organics would serve a similar purpose as anaerobic digestion but represent a more robust option.

Publications, Patents, Presentations, Awards, and Commercialization – Characterization

- ▶ Characterization Results published in Biomass and Bioenergy (March, 2015)
- ▶ Journal peer-reviewer comments extremely positive (selected comments shared below)



Biomass and Bioenergy

Volume 74, March 2015, Pages 162–171



Characterization of the aqueous fractions from hydrotreatment and hydrothermal liquefaction of lignocellulosic feedstocks

Ellen Panisko , Thomas Wietsma , Teresa Lemmon , Karl Albrecht , Daniel Howe 

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Received 3 October 2014, Revised 31 December 2014, Accepted 12 January 2015, Available online 6 February 2015

“The work addresses a significant knowledge gap in the literature related to the aqueous phases from thermochemical processes.”

“The paper contains very useful (and timely) information on detailed analysis of these aqueous streams in both the context of potential contaminants during upgrading and the question of how to dispose of the effluent or for chemical recovery.”

“Very good GC and HPLC work! Quantification performed the way it should be.”

“It is an excellent work with significant results.”

“The authors provide important chemical characterization of the aqueous fraction of HTL and HDO/pyrolysis oil liquid products that are generally considered waste and ignored. The manuscript is well-written and thorough.”

Publications, Patents, Presentations, Awards, and Commercialization – Catalytic Conversion

■ Presentations

1. Karthikeyan K. Ramasamy, Karl O. Albrecht, Mark A. Gerber, Matthew Flake. *Organic Components Produced in Biomass Liquefaction Process Over HZSM-5*. Poster presented at TC Biomass on August 30, 2013. Chicago, IL.
2. Karthikeyan K. Ramasamy, Karl O. Albrecht, Alan R. Cooper, Becky L. Thompson, Mark A. Gerber, Robert A. Dagle, Guo-Shuh (John) Lee, and Matthew Flake. *Upgrading of Organic Compounds in the Aqueous Phase Produced by Biomass Direct Liquefaction Processes*. Oral presentation given at the 246th ACS National Meeting September 12, 2013. Indianapolis, IN.
3. Karl O. Albrecht, Alan R. Cooper, John G. Frye, Yunhua Zhu, Donghai Mei, Suh-Jane Lee, Teresa L. Lemmon, Heather M. Job. *Catalytic Conversion of Organic Compounds in the Aqueous Phase Produced by the Hydrothermal Liquefaction of Terrestrial Biomass*. Oral presentation delivered at TCS2014 on September 2, 2014. Denver, CO.
4. Karl O. Albrecht, Alan R. Cooper, John G. Frye, Suh-Jane Lee, Robert A. Dagle, Vanessa M. Dagle. *Condensed Phase Ketonization of Organic Acids Produced by the Hydrothermal Liquefaction of Lignocellulosic Biomass*. Oral presentation accepted for delivery at AIChE 2015 Spring Meeting April 27, 2015. Austin, TX.
5. Karl O. Albrecht*, Alan R. Cooper, John G. Frye, Robert A. Dagle, Vanessa M. Dagle. *Condensed Aqueous Phase Ketonization of Organic Acids Produced by the Hydrothermal Liquefaction of Lignocellulosic Biomass*. Oral presentation submitted for the NACS North American Meeting June, 2015. Pittsburgh, PA
6. Donghai Mei, Karl O. Albrecht, Alan R. Cooper, Vanessa Dagle and Robert Dagle. *Effects of Solvents on Acetic Acid Ketonization over Zirconia Catalysts – A Combined Theoretical and Experimental Study* Oral presentation submitted for the NACS North American Meeting June, 2015. Pittsburgh, PA

■ Invention disclosure: Catalytic conversion of organic acids to ketones in the condensed aqueous phase. September 2014.

Publications, Patents, Presentations, Awards, and Commercialization – Steam Reforming

■ Presentations

1. Xing R, RA Dagle, VMC Lebarbier, KO Albrecht, DL King, and MA Gerber. 2013. "Steam Reforming the Aqueous Phase Components Produced in Direct Liquefaction Processes ." Poster presented by Robert Dagle at TCBIomass, Chicago, IL on September 3, 2013. PNNL-SA-98038.
2. Xing R, RA Dagle, VMC Lebarbier, KO Albrecht, DL King, and MA Gerber. 2013. "Steam Reforming the Aqueous Phase Components Produced in Direct Liquefaction Processes ." Presented by Rong Xing at 246th American Chemical Society National Meeting, Indianapolis, IN on September 12, 2013.

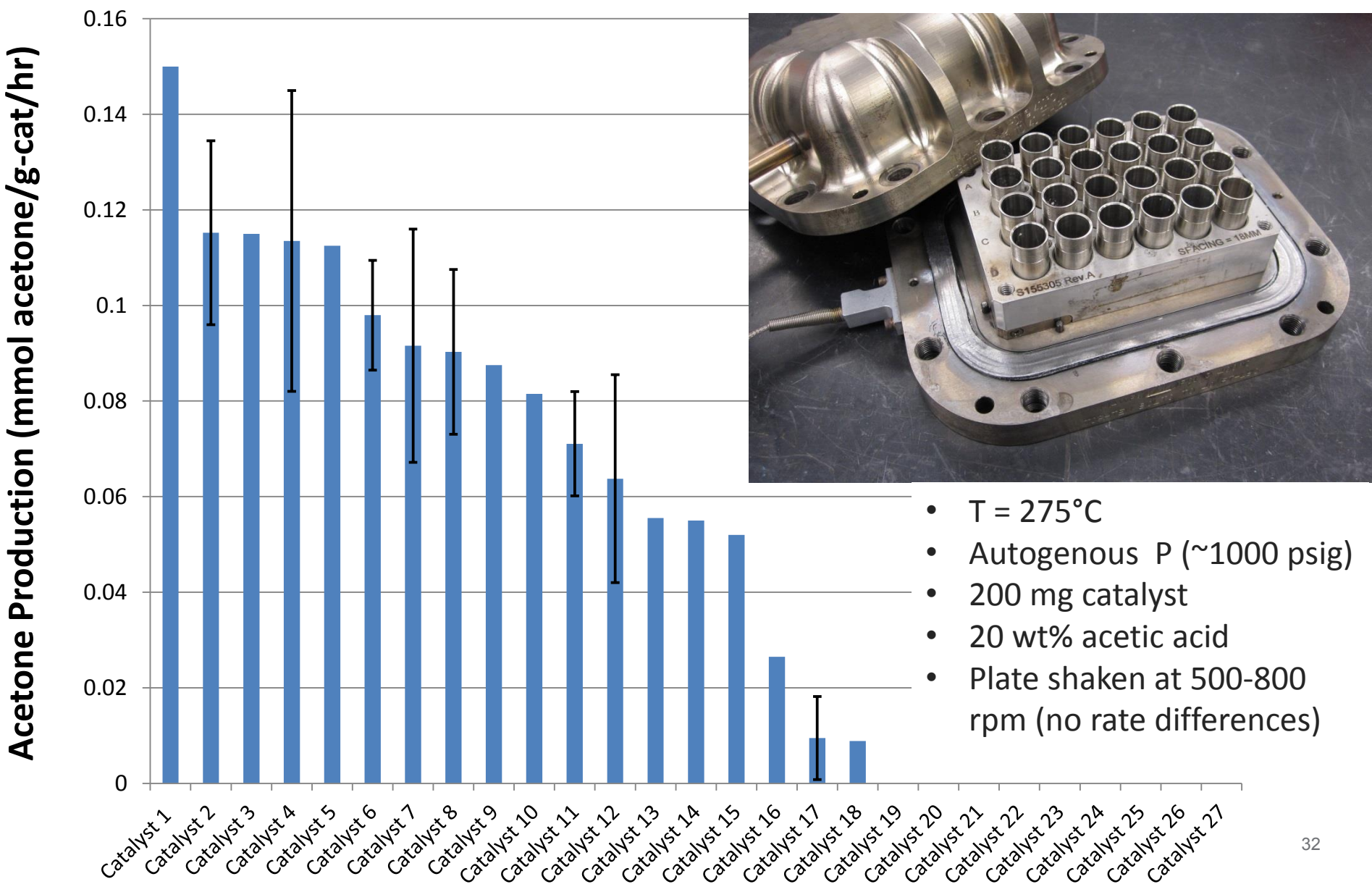
■ Publications

1. Donghai Mei,* , Vanessa Dagle, Xing Rong, Karl O. Albrecht, Robert A. Dagle. "Steam Reforming of Ethylene Glycol over MgAl₂O₄ Spinel Supported Metal Catalysts: Combining Theoretical Modeling with Experiments." *To be submitted to ACS Catalysis*.
2. Rong Xing, Robert Dagle, Vanessa Lebarbier Dagle, Chinmay Deshmane, Karl O. Albrecht, and Dave L. King. "MgAl₂O₄-Supported Catalysts for Steam Reforming Aqueous Oxygenates Produced in Direct Liquefaction Processes ." *In preparation*.



Additional Technical Slides

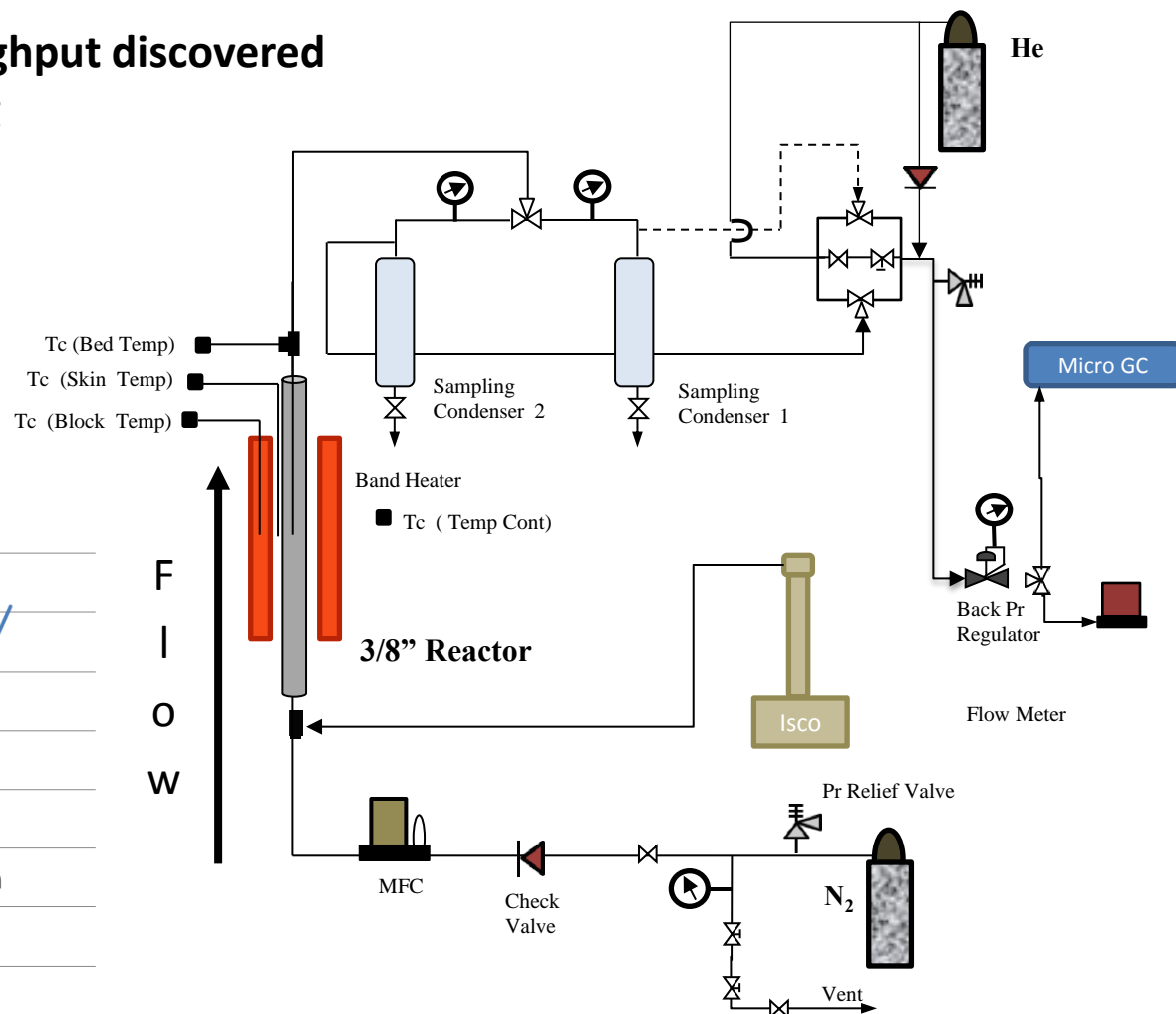
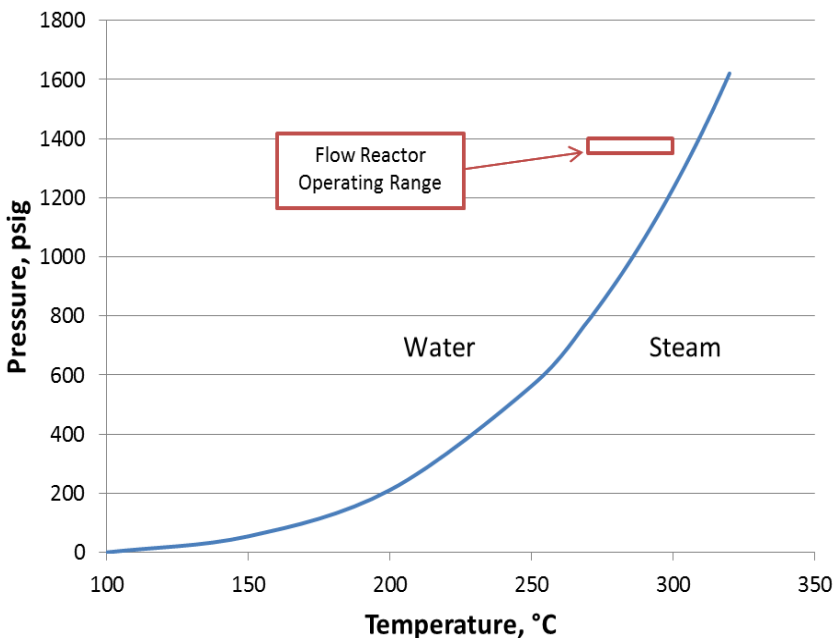
Catalytic Conversion High Throughput Screening for Acetone Production Catalysts



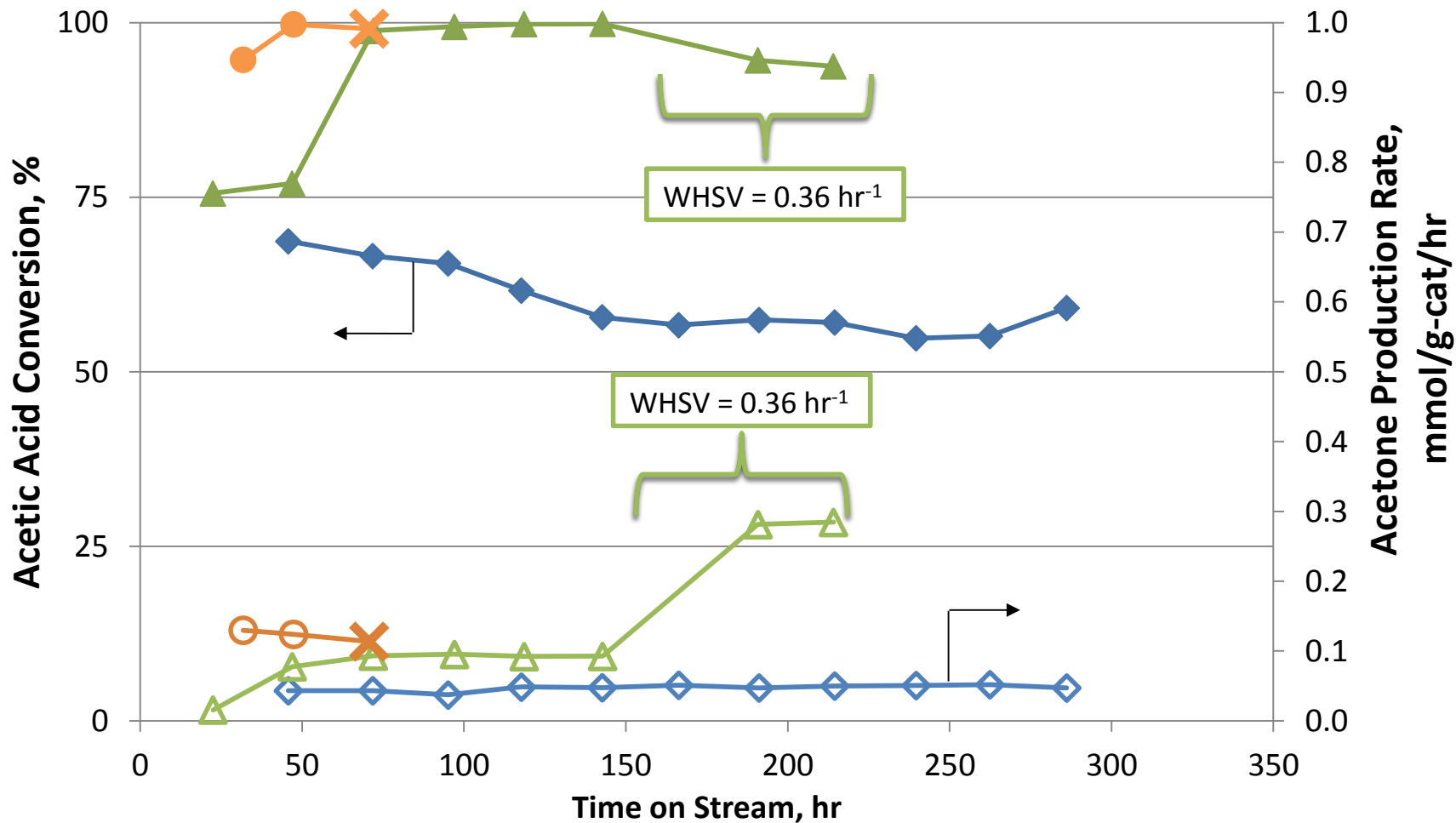
Catalytic Conversion Upflow Fixed-Bed Reactor Testing Method

Activity comparison of high-throughput discovered catalysts via fixed-bed flow testing

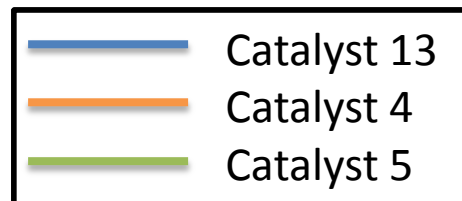
300°C
1350-1400 psig
1.0-5.0 g catalyst
0.12-0.37 g feed/g-catalyst/hr (WHSV)
10% - 22% acetic acid/water



Selected Catalyst Comparison Upflow Fixed-Bed Reactor Testing



300°C, 1350-1400 psig
WHSV = 0.12 hr⁻¹
10% Acetic Acid/H₂O



Effect of Concentration with Model Acetic Acid $\text{La}_2\text{O}_3/\text{ZrO}_2$ Catalyst

	10% acetic acid	22% acetic acid
Time on Stream, Hr	214	76
Acetic Acid Conversion	94%	52%
Acetone produced (mmol/g-cat/hr)	0.28	0.32
Acetic acid consumption (mmol/g-cat/hr)	0.55	0.71
Selectivity (2*acetone/acetic acid conv)	102%	90%
Carbon Balance	97%	92%

**Acetone production appears to be 0 order
with respect to acetic acid concentration**

300°C, 1350-1400 psig, WHSV = 0.36 hr⁻¹