NREL
Transforming ENERGY

Gas Phase Selective Partial Oxidation of Lignin for Co-products from Biomass Conversion

WBS# 2.3.1.501– 33404

Tuesday, March 9, 2021
Biochemical Conversion/Lignin Session
PI: Matthew Yung - NREL

Goal Statement

Goal – Produce phenolic co-products from a biorefinery lignin stream by developing lignin pyrolysis coupled with selective catalytic oxidation to create a valuable, diverse revenue stream to facilitate BETO's $2.50/GGE cost targets

- *Focus on high value **phenolic products** with **large markets** and potential for bio-adoption (support >200 biorefineries at 2000 tonne/day biomass)*

Outcome: A process-agnostic technology to create a revenue stream by producing phenols from biorefinery lignin, thereby enabling cost-competitive fuel production

Relevance

Conversion Technology	Benchmark on Commercial Catalyst*	NREL State of Technology *		Long-Term Target	R&D Challenge
Lignin Pyrolysis	Char Yield 33%	25-50% char	→	15-25% char	Reduce foaming; increase heat transfer; improve operability and gas yields to phenolics
Partial Oxidation of Gas Phase Lignin Pyrolysis Products	Simple Phenols Yield 8%	15% yield (Go/No-Go 10%)	→	25% yield	Tune catalyst metal-oxygen bond strength and process parameters; Balance catalyst acidic and alkylation sites with oxidation sites
	Estimated reduction in MFSP $0.25/GGE*	Reduction of >$0.60/GGE*	→	Reduction of ≥$1.35/GGE*	Improve economics by integrating TEA process design with catalyst development and reaction testing

Quad Chart Overview

Timeline

- Project start date: 10/1/2017
- Project end date: 9/30/2020*
- Percent complete: 100%

Budget

	Pre FY20 Costs	FY20 Costs	FY21 Remaining Carryover
DOE Funding	$726K	$304K	$125K

Partners/Collaborators

- **Industry Partners:** Sweetwater Energy, Renmatix, Johnson Matthey, Sumitomo Bakelite, BASF, Ensyn, West Fraser Timber
- **NREL BETO Projects**: Co-Products Production, Pretreatment & Process Hydrolysis, Biochemical Platform Analysis, Catalytic Fast Pyrolysis
- **BETO ChemCatBio Consortia**: Advanced Catalyst Synthesis and Characterization (ACSC), Consortium for Computational Physics and Chemistry (CCPC)

BETO MYP Barriers Addressed

Ct-C. Process Development for Conversion of Lignin
Ct-F. Increasing the Yield from Catalytic Processes
Ct-K. Developing Methods for Bioproduct Production
Ot-B. Cost of Production

Developing catalysts and processes to convert lignin to high value phenolic compounds – diversifying biorefinery revenue streams and thereby reducing the MFSP from biorefineries

Objective

Produce phenolic co-products from a lignin stream by developing selective oxidation catalysts for lignin pyrolysis vapors to facilitate BETO's $2.50/GGE cost targets.

End of Project Goal (FY20)

- Demonstrate gas phase partial oxidation of lignin using a bench-scale reactor:
  - >10% phenolics yield for estimated impact of >$0.40/GGE reduction in MFSP
  - Perform detailed analysis of condensed phenols by distillation, GC/MS, GPC, and NMR

1. Overview

1. Project Overview (1 of 2)

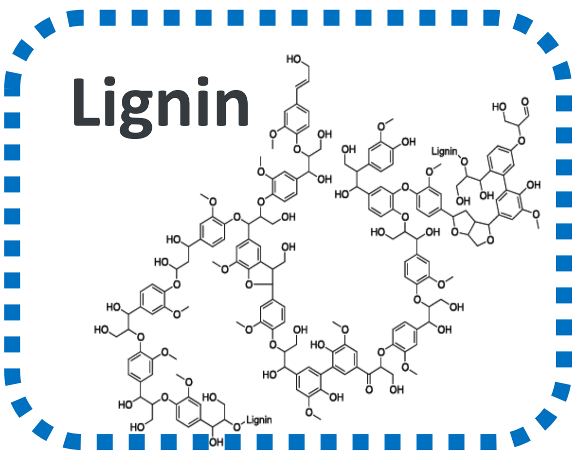
Context and History:

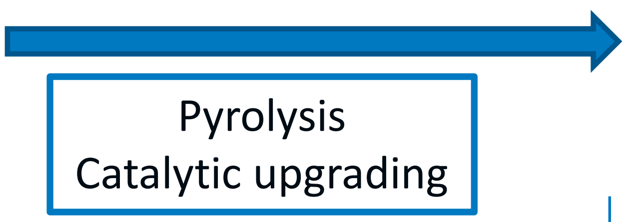
- Project in response to 2017 BETO peer review feedback
  - Opportunity for catalytic pyrolysis to upgrade specific biomass fractions (lignin, cellulose, hemicellulose) to make a narrower product slate

Project Goals:

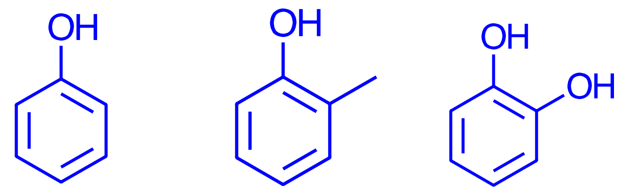
- Upgrade lignin to simple phenols by developing catalysts to convert lignin pyrolysis vapors via oxidative cleavage
  - Simple phenols used in polycarbonates, epoxide resins, and plastics
  - >10% yield to phenolics on bench-scale by FY20

Large market sizes for phenolics could support >200 biorefineries at 2000 tonne/day biomass





Oxygenated Aromatics (Simple Phenols)

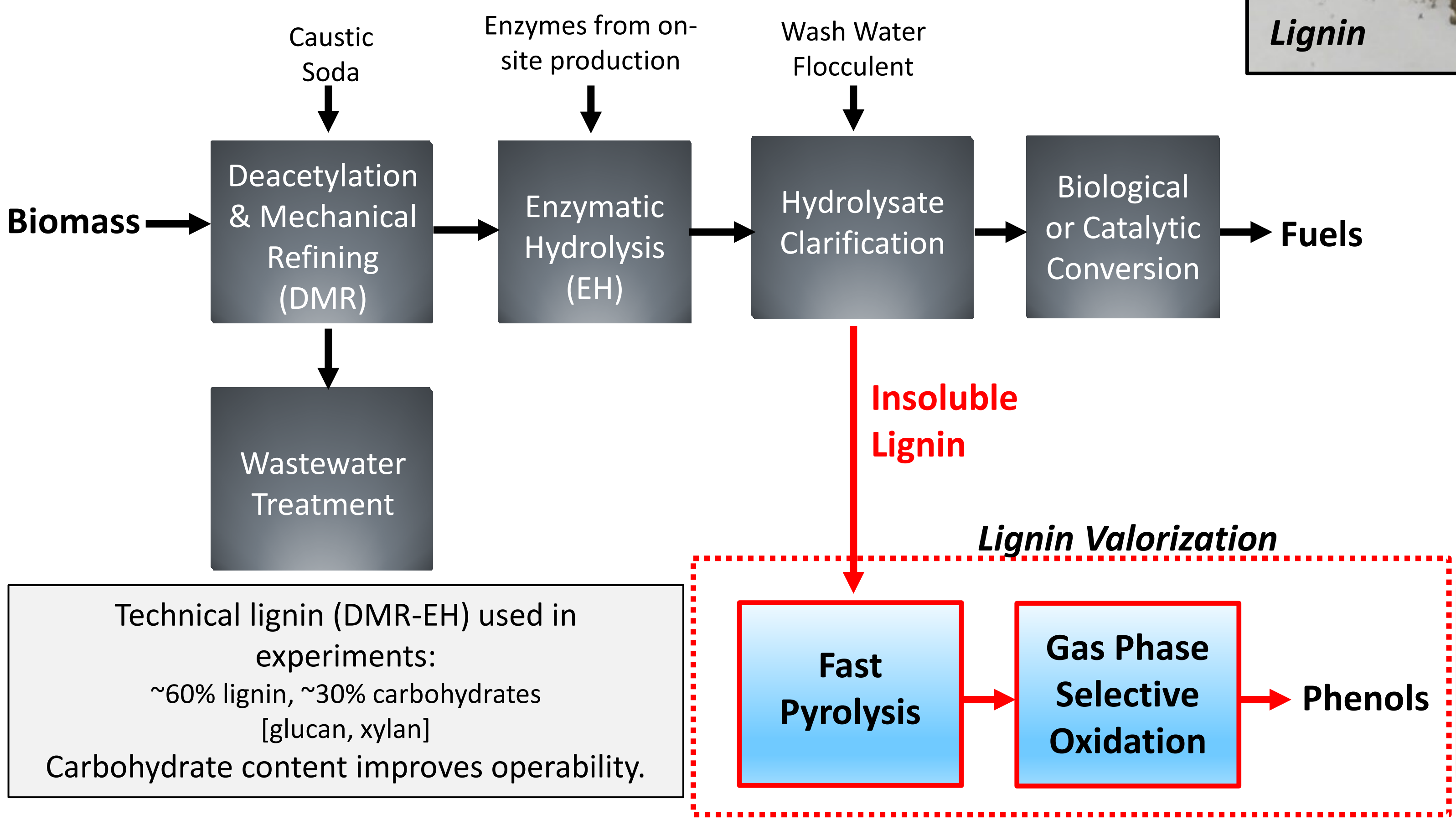


	Phenol	2-Cresol	Catechol
Price ($/kg)	$1-2/kg	$3-5/kg	$5-7/kg
Market Size (kTA)	11,400	3,400	45

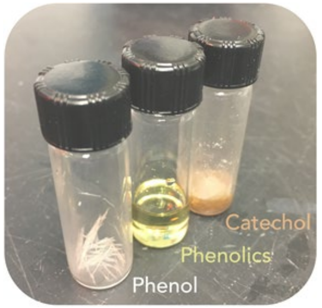
Carvajal, J.; Byrne, D. *Chemical Economics Handbook Phenol (686.500)*, IHS, 2014.

Simplified Process Flow Diagram

1) Convert C_5/C_6 sugars from biomass to fuels
2) Produce phenols by thermochemically converting lignin pyrolysis vapors via selective oxidation



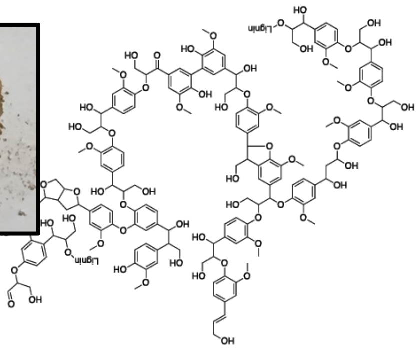
Technical lignin (DMR-EH) used in experiments:
~60% lignin, ~30% carbohydrates [glucan, xylan]
Carbohydrate content improves operability.



2. Approach - Technical

2. Technical Approach (1 of 4)

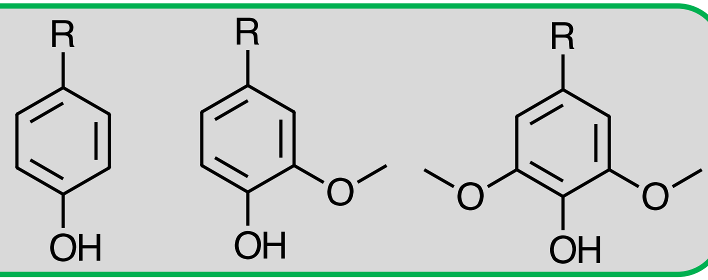
Create phenols from catalytic oxidation and avoid carbon loss to undesirable products.



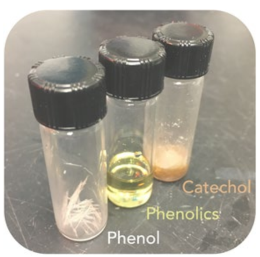
LIGNIN FROM BIOCHEM. PROCESS

Pyrolysis

LIGNIN PYROLYSIS PRODUCTS

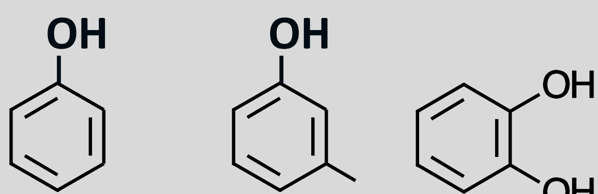


Catalytic partial oxidation



SIMPLE PHENOLS

phenol	cresol(s)	catechol



phenol	cresol(s)	catechol
\$1-2/kg	\$3-5/kg	\$5-7/kg
11 Mtons/y	3 Mtons/y	0.05 Mtons/y

Char
25-60 wt%
(recalcitrant C-C linkages in lignin)

CO and CO_2
>10 wt%
(undesired oxidation products)

Challenges – Phenol yield is critical for economics; catalyst regeneration; lignin feeding on large systems

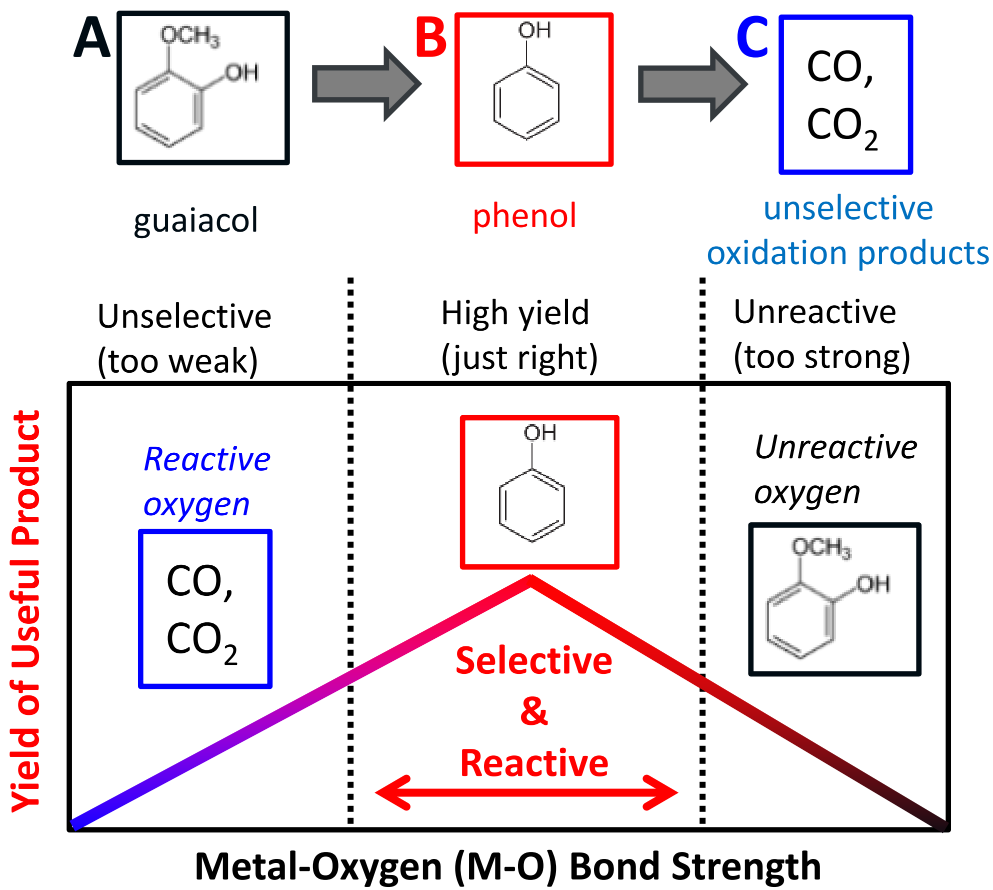
2. Technical Approach (2 of 4)

Synthesize catalysts with varying surface properties:

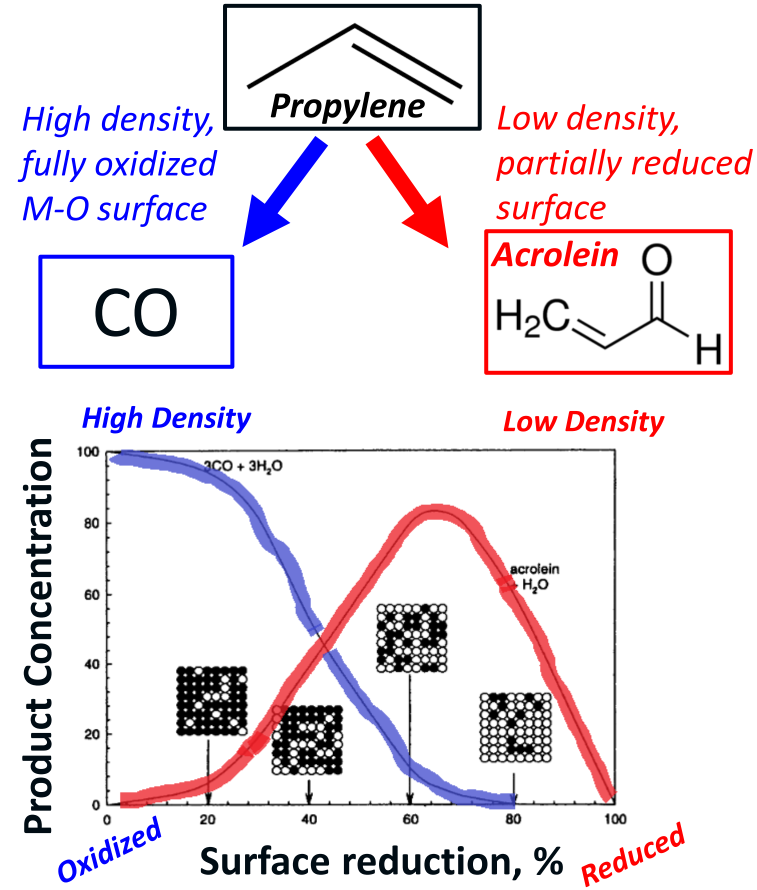
(1) Metal-oxygen bond strength **(2) Active site density**

-Important for parameters for selective oxidation catalysts

1. Metal-oxygen Bond Strength

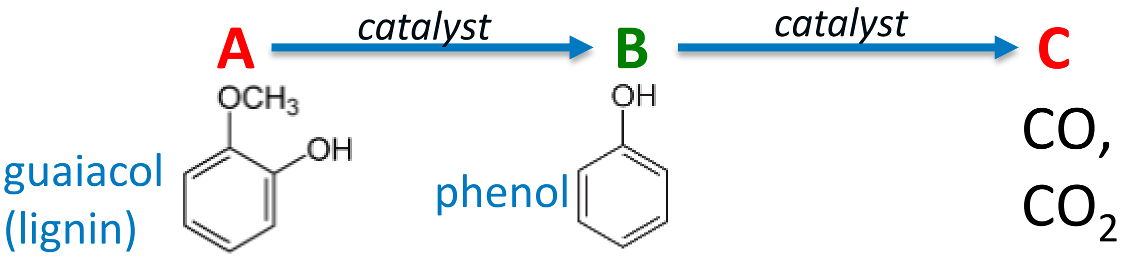


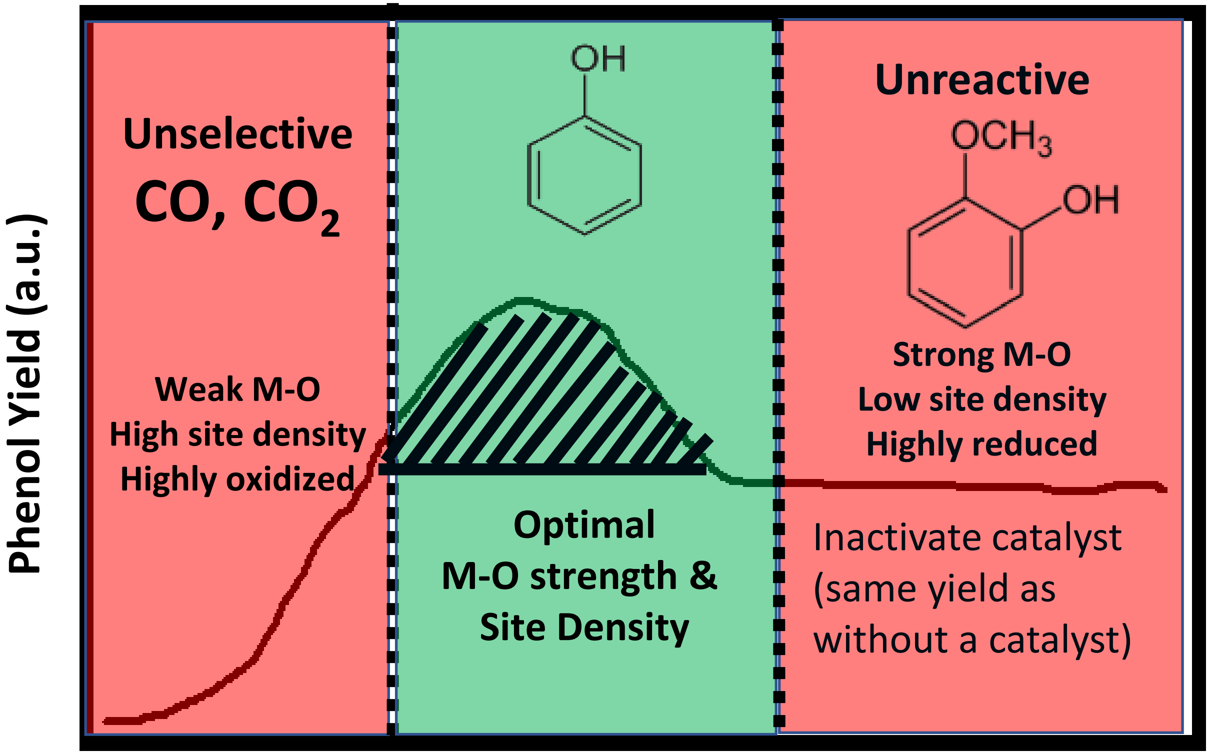
2. Active Site Density



*Grasselli, *Top. Catal* 2002, 79-88. *Chen, J. Catal, 2002, 35-42.*

Tailor catalyst by changing surface properties to maximize yield of desired product (phenols).





Catalyst Surface Properties

(1. Increasing Metal-Oxygen Bond Strength, 2. Decreasing Site Density)

Critical Success Factors

Achieving high phenolic yields is most critical to TEA

Challenges

- High yield and selectivity;
- Lignin feeding on large systems;
- Catalyst regeneration

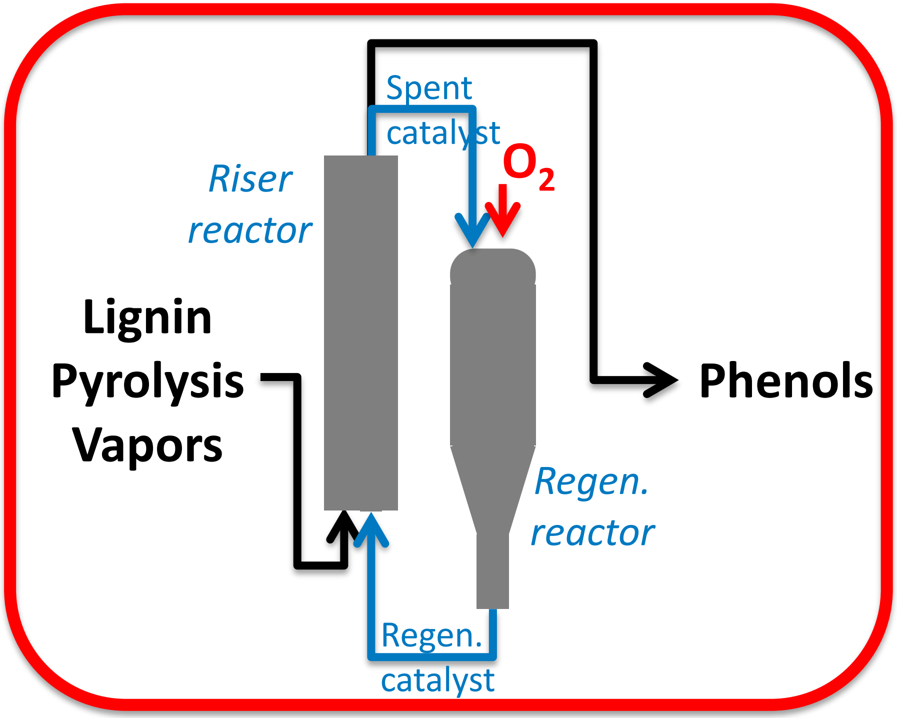
Regeneration: Closing the Catalytic Cycle

Two process options to regenerate and replenish catalyst surface oxygen:

1. Chemical looping (circulating catalyst with regeneration in separate vessel)
2. Co-feed oxidant (O_2 or CO_2)

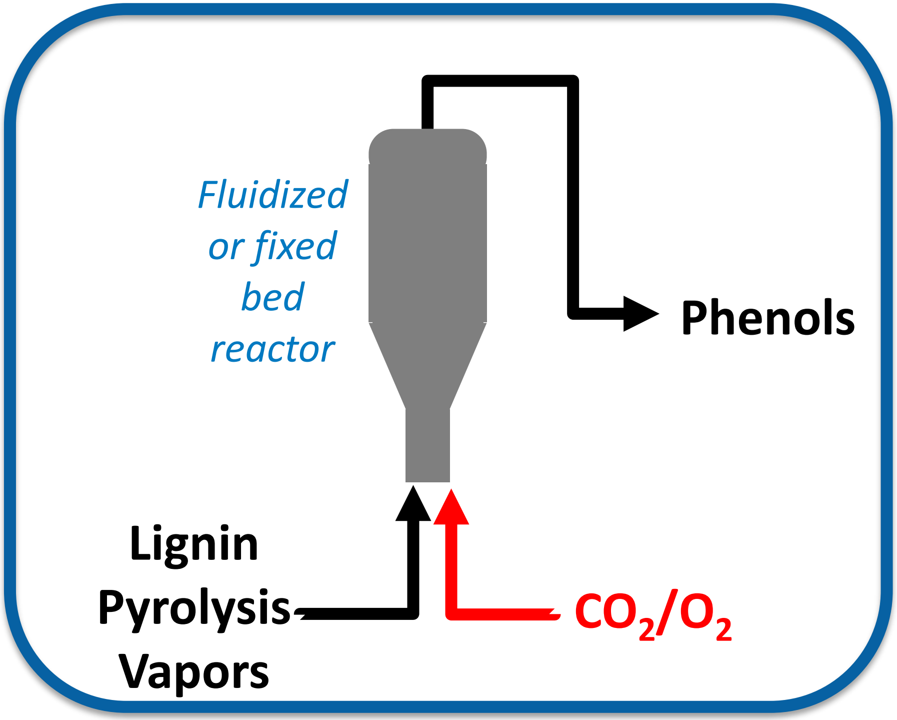
Chemical Looping

(Riser & regeneration reactors; used in industry – fluidized catalytic cracker)



Co-Feed Oxidant

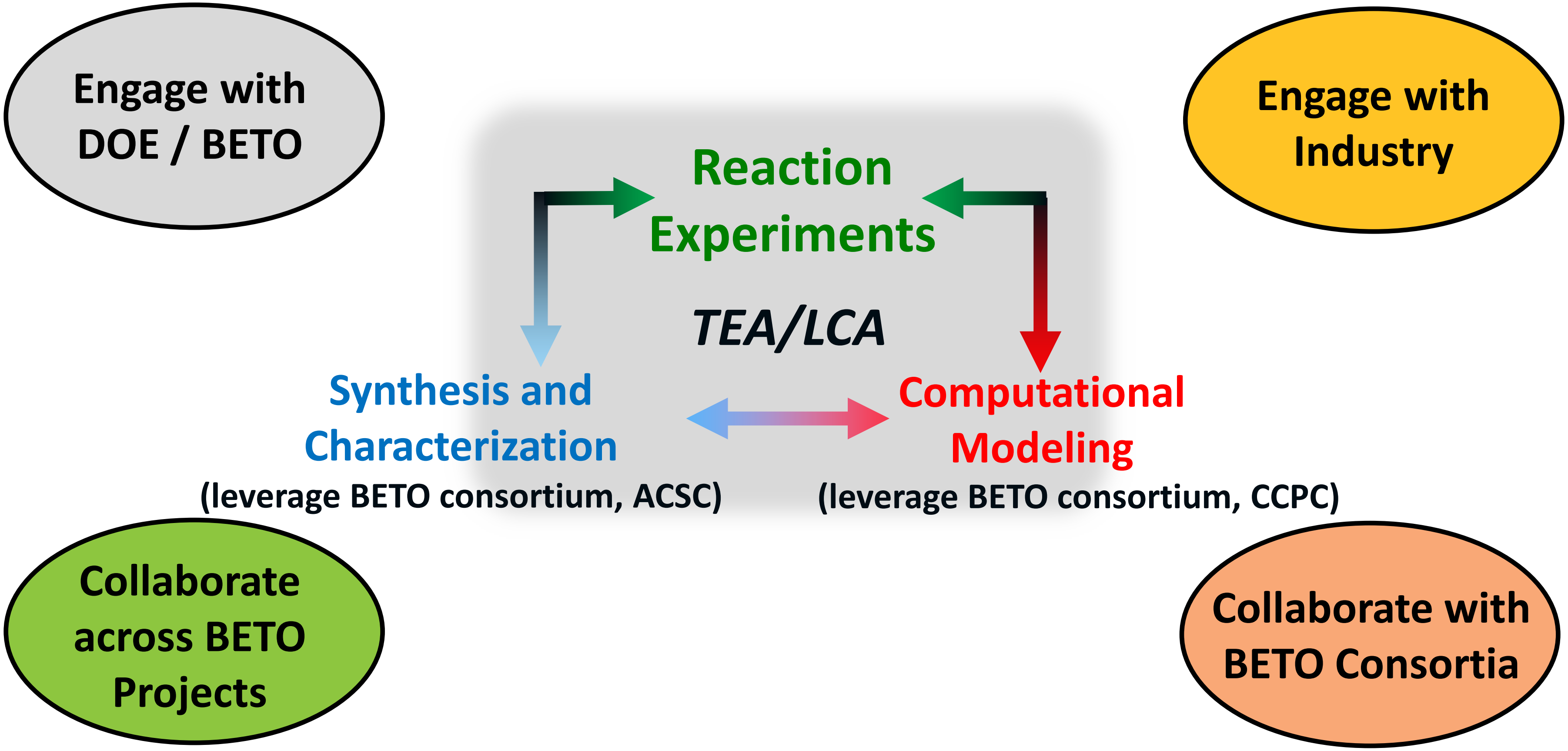
(Fluidized or fixed-bed reactor)



1. Overview
2. Approach - Technical
3. Management
4. Progress and Accomplishments
5. Impact

3. Management

3. Management Approach: Task Structure (1 of 4)



- Performance Advantage Bioproducts
- Catalytic Fast Pyrolysis
- Technoeconomic Analysis
- Separations

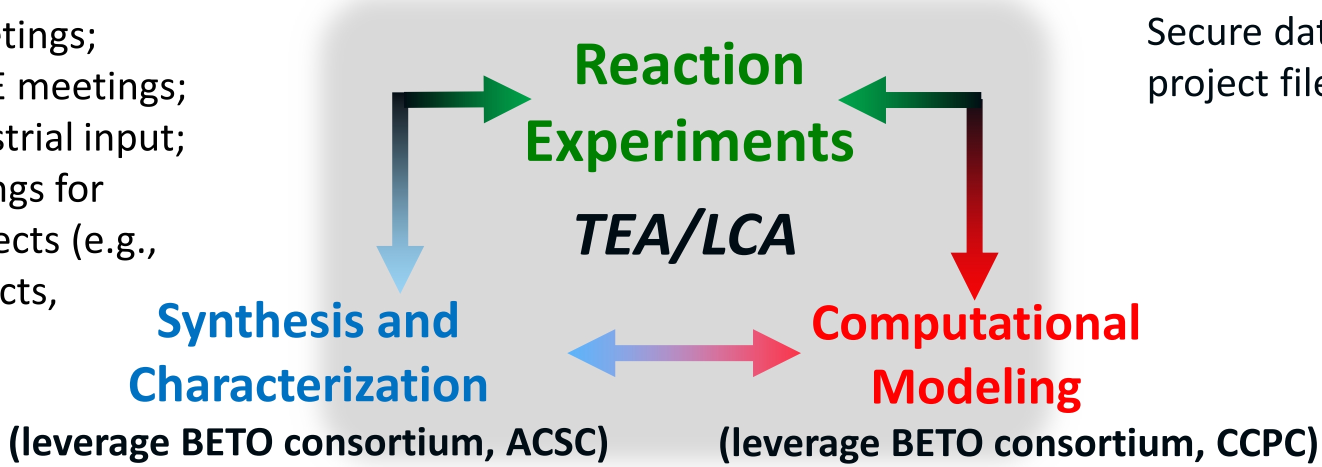
- ACSC - Advanced Catalyst Characterization & Synthesis
- CCPC - Consortium for Computational Physics and Chemistry

Go/No-Go – Focused on critical success factor – yield of phenolics:
"Demonstrate ≥10% yield of phenolics on lab-scale…" March 2019

- **Surpassed goal (achieved 15% phenol yield on lab-scale)**

Project Communication– Biweekly meetings; quarterly DOE meetings; ongoing industrial input; attend meetings for adjacent projects (e.g., CFP, co-products, separations)

Data Management – Secure data folders for all project files



Interdisciplinary Team Members – Expertise in reaction engineering, characterization, synthesis, computation, TEA/LCA, and scale-up

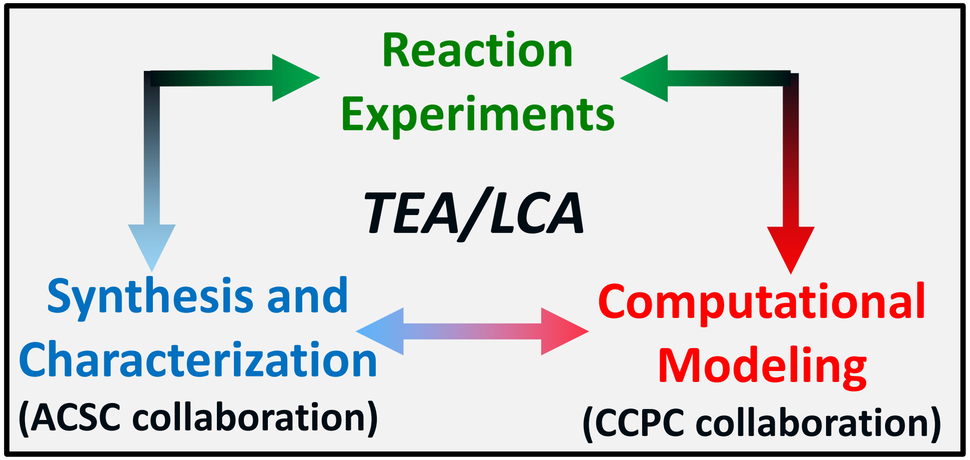
Leverage BETO Projects– Collaborate and leverage BETO ChemCatBio enabling technology consortia for computation (CCPC) and characterization (ACSC), CFP, Performance Advantaged Bioproducts, TEA

Integrated Approach– Development is accelerated by an iterative, multi-facetted approach to R&D challenges

3. Management: Technical Approach (3 of 4)

Flow Chart for Managing Project Activities

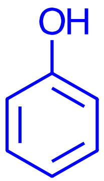
1) Baseline lignin pyrolysis (no catalyst)
2) Benchmark commercial catalyst
3) Use computation to guide initial catalyst synthesis/selection
4) Prepare materials of varying metal-oxygen strength and site density
5) Test catalysts with model compounds and whole vapors
6) Use experimental data with TEA/LCA models
7) Iterate and improve based on findings



8. Scale-up catalyst and demonstrate on bench-scale

3. Management: Risk Assessment/Mitigation (4 of 4)

Project Risks and Mitigation Strategies

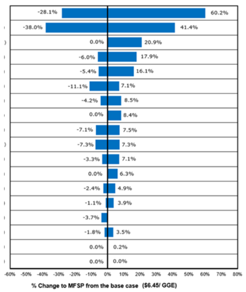


Focus on increased product yield

Carbon Efficiency
Concerted effort towards ↑yield via catalyst/process improvement and pyrolysis to ↓char, thus enabling cost goals

Process Economics
Establish performance targets and develop sensitivity analysis to identify the most-impactful, largest cost reduction parameters

$$$



Economic sensitivity

Equipment failure and staffing disruption
Develop redundancies in key capabilities and operations (e.g., reactor, analytical, characterization, industrial lignin supply) to mitigate disruption to project progress

Contaminants Effects with Real Process Lignin
Utilize industrially-sourced, *real process lignin* (not model compounds) to reduce risk of unknown contaminant and material impacts

Commissioning of micro-reactor for catalyst site titrations and kinetic studies

Process lignin samples from industry partners

1. Overview
2. Approach - Technical
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3. Progress and Accomplishments

4. Progress / Accomplishments (1a of 8)

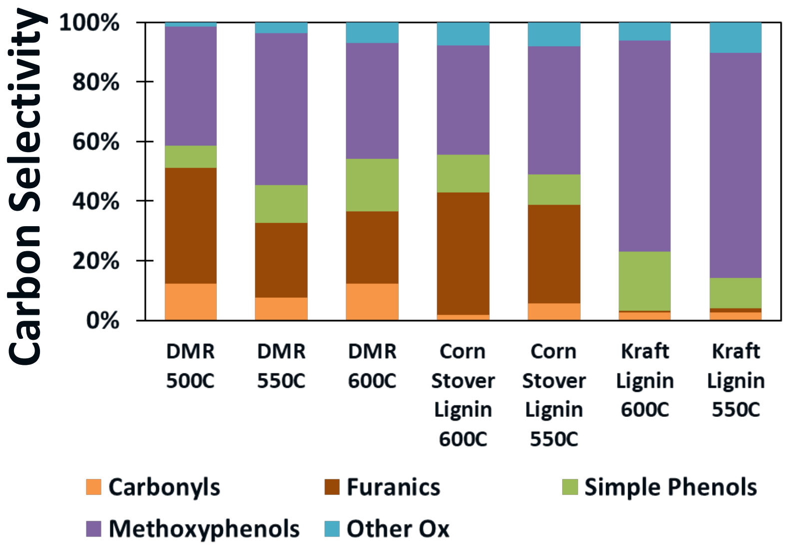
1. Baseline Pyrolysis: Examine various types of lignin and pyrolysis conditions and their effects on product yields to establish baseline condition(s) and feedstock(s) for experiments.

4. Progress / Accomplishments (1b of 8)

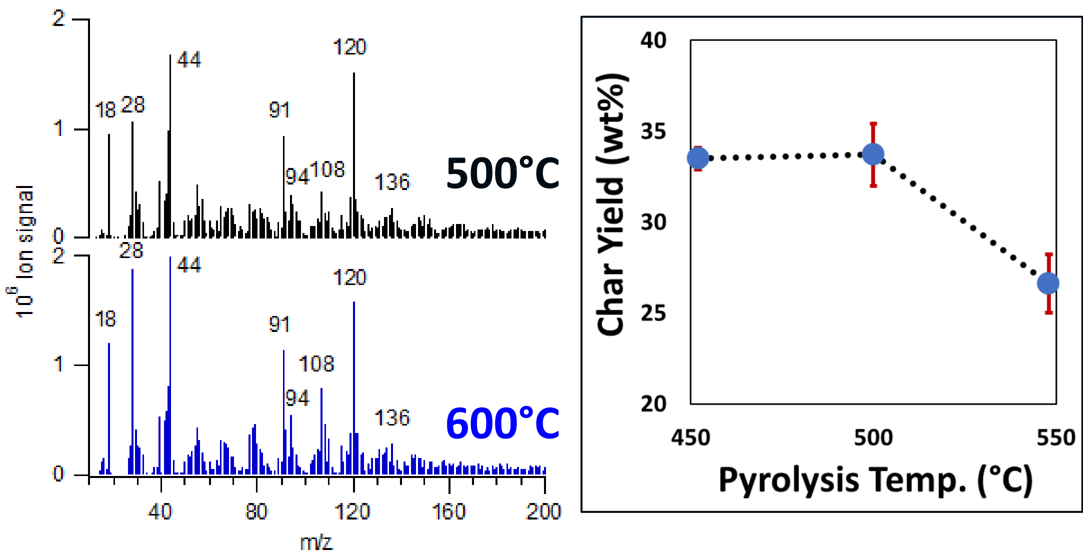
1. Baseline Pyrolysis: Examine various types of lignin and pyrolysis conditions and their effects on product yields to establish baseline condition(s) and feedstock(s) for experiments.

- **Pyrolysis testing of multiple lignins (different processes and biomass sources)**
  - **DMR-EH** (corn stover), corn stover, pine mixed softwoods, Sweetwater, Renmatix, Kraft
  - GC/MS analysis of condensed products
  - MBMS of gaseous products prior to condensation

Pyrolysis Products from Various Lignin Types



Mass spectra and char yields of DMR-EH lignin pyrolysis vapors at varying pyrolysis temperatures



1. Baseline Pyrolysis

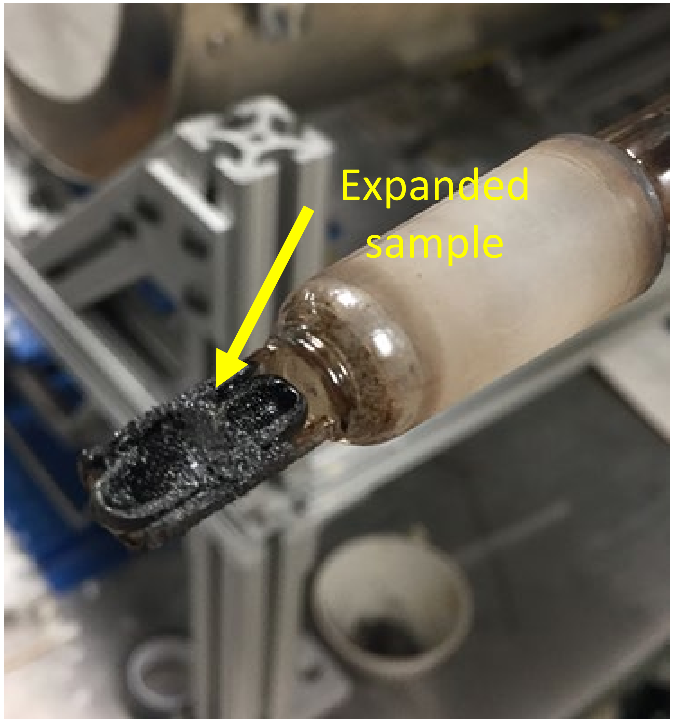
Lignin Pyrolysis (high lignin content, >90%)

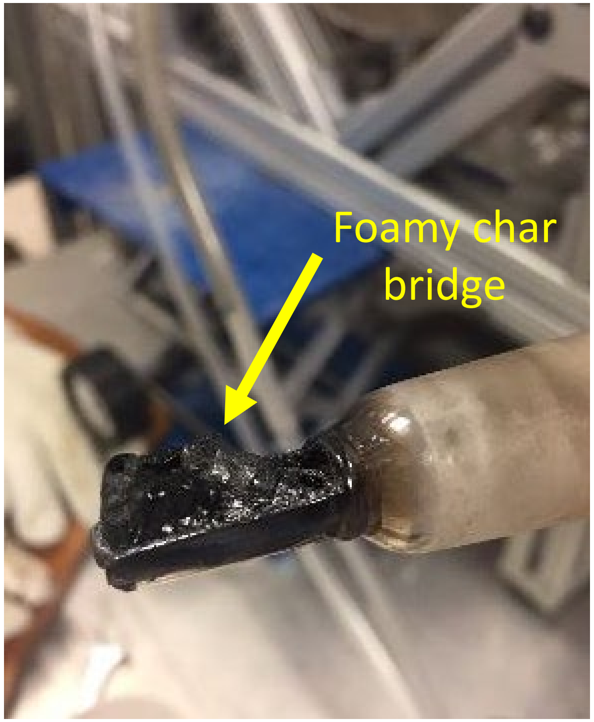
Before pyrolysis

Lignin rests nicely in quartz boat

After pyrolysis

Foamy, sample expansion, forms a char bridge spanning the sample holder and encapsulating the quartz boat



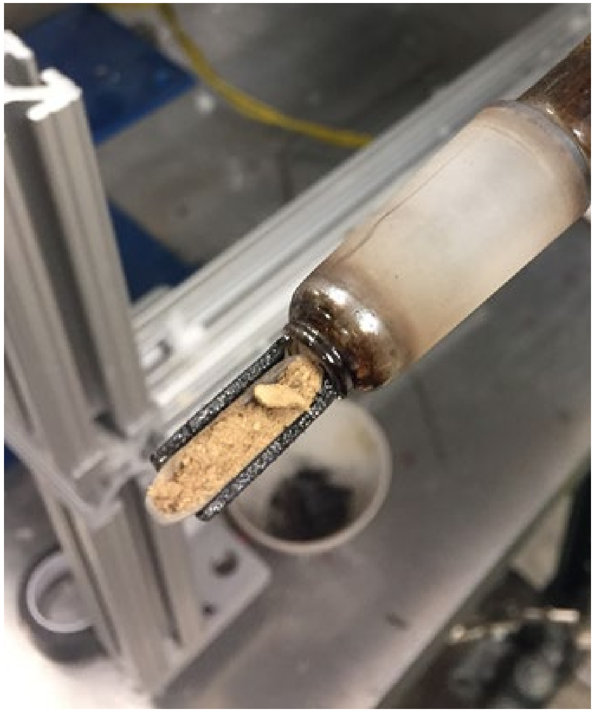


1. Baseline Pyrolysis

DMR Lignin Pyrolysis (60% lignin content)

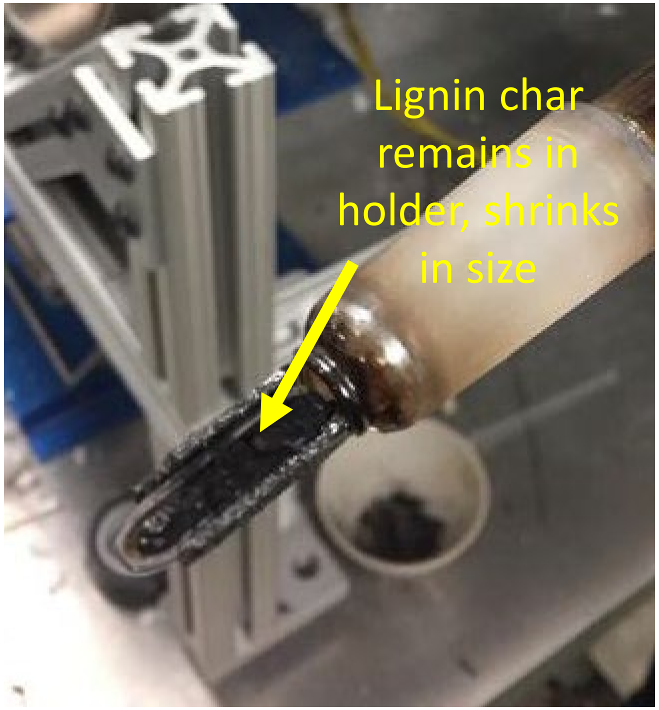
Before pyrolysis

Lignin rests nicely in quartz boat

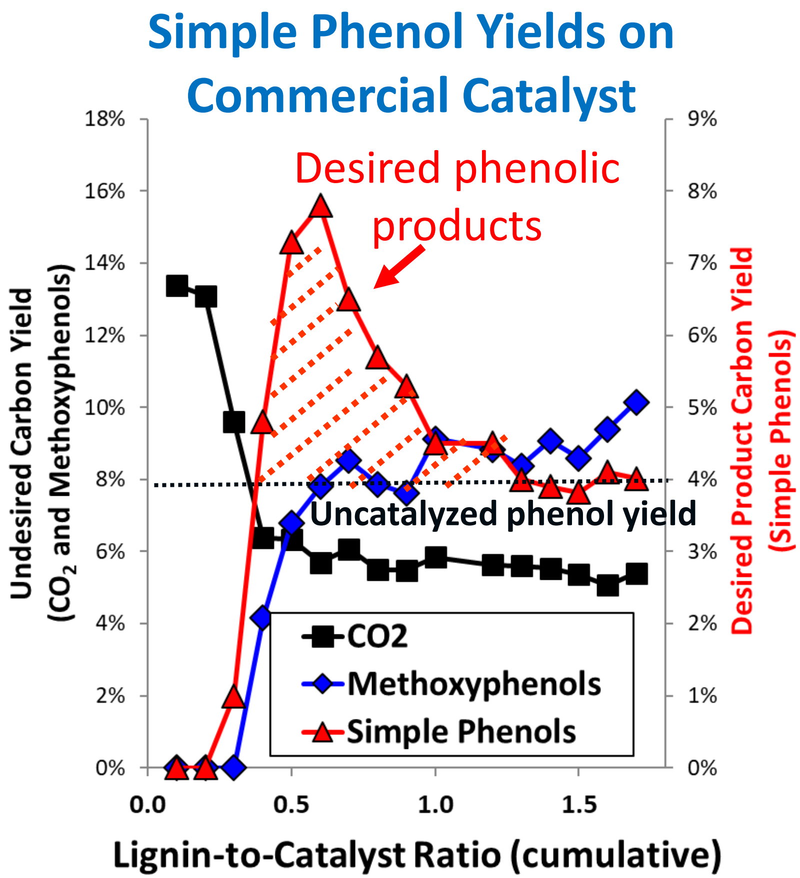


After pyrolysis

No expansion, char remains nicely situated within sample holder



2. Benchmark Commercial Catalyst: A commercial vanadia oxidation catalyst was evaluated for oxidation of lignin pyrolysis vapors to establish a benchmark for phenol yields to compare the NREL-developed catalysts.



Reaction conditions: Pyrolysis/catalysis of 600°C/ 500°C DMR-EH lignin over V_2O_5 to cumulative lignin:biomass of 1.8.

Baseline carbon yields to simple phenols from DMR-EH lignin pyrolysis:	
4%	**Uncatalyzed (pyrolysis-only)**
8%	**Commercial catalyst benchmark** *(13% based on lignin content of DMR-EH residue)*

- Concept of lignin oxidative conversion to phenolic successfully demonstrated using whole lignin pyrolysis vapors

3. Computational Catalysis: Leveraging on-going BETO modeling work with in-project expertise to provide understanding of isolated sites. Reaction pathway for conversion of guaiacol to simple phenols investigated over isolated vanadium species.

BETO consortium

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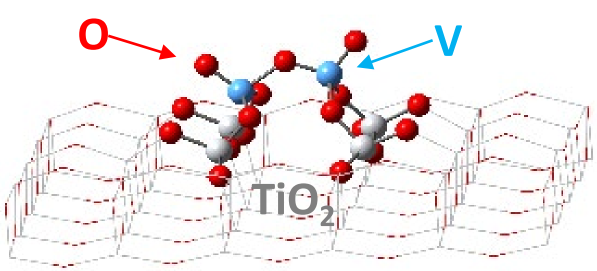
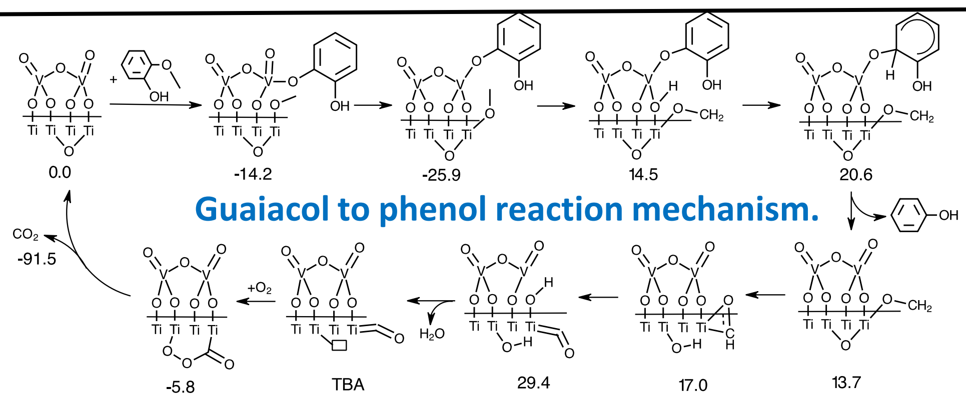
Bond strengths (kcal mol[-1]) for a lignin monomer.

- Understand bond strengths and opportunities for selective bond cleavage.



Molecular model of V_2O_5/TiO_2: V (blue), O (red), Ti (white) on TiO_2 support.

- Develop models of V_2O_5-supported catalysts on various metal oxides (e.g., TiO_2, SiO_2, Al_2O_3, ZrO_2) and determine relative V-O bond strengths.

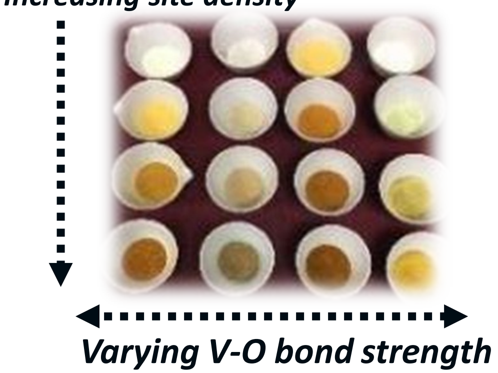


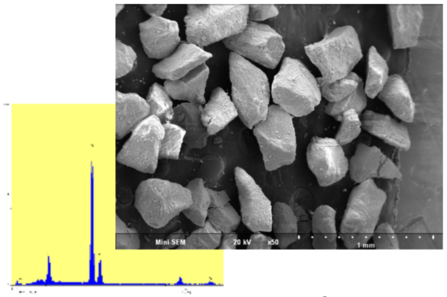
Guaiacol to phenol reaction mechanism.

- Explore mechanism(s) for surface reactivity. Established reaction pathway catalytic conversion of guaiacol to phenol was established over isolated vanadium species supported on TiO_2

4. Synthesis and Characterization of Catalysts: Successfully synthesized and characterized lignin catalysts with varying metal-oxygen bond strength, active site densities, and molecular structures.

Optical and SEM images of NREL-synthesized lignin oxidation catalysts

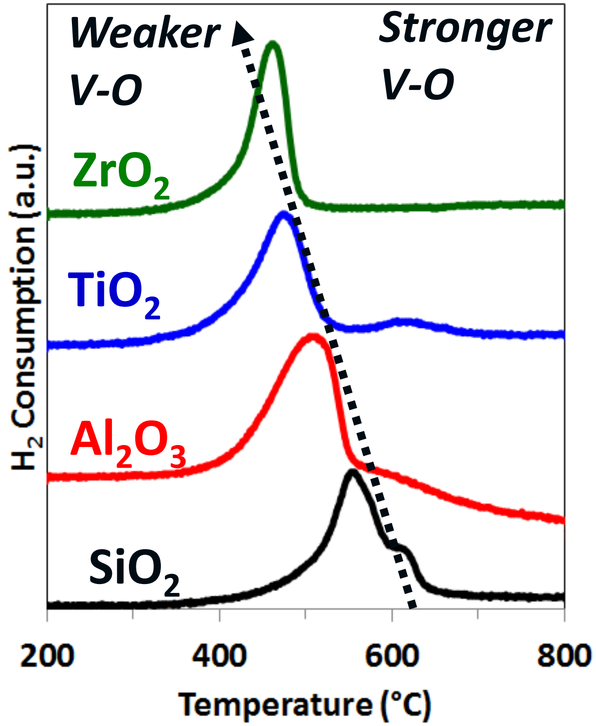




SEM EDS of V_2O_5/TiO_2

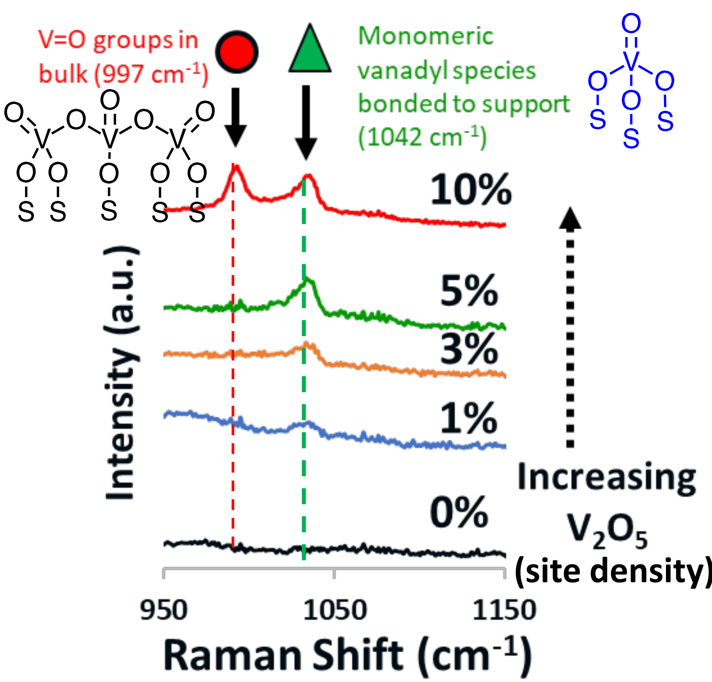
Metal-oxygen bond strength can be tailored.

H_2 temperature-programmed reduction (TPR) of 10% V_2O_5 on different supports showing varying M-O bond strengths



Molecular species change with changing site density.

Laser Raman Spectroscopy identified transition from isolated to polymeric vanadyl species with increasing vanadium loading and site density

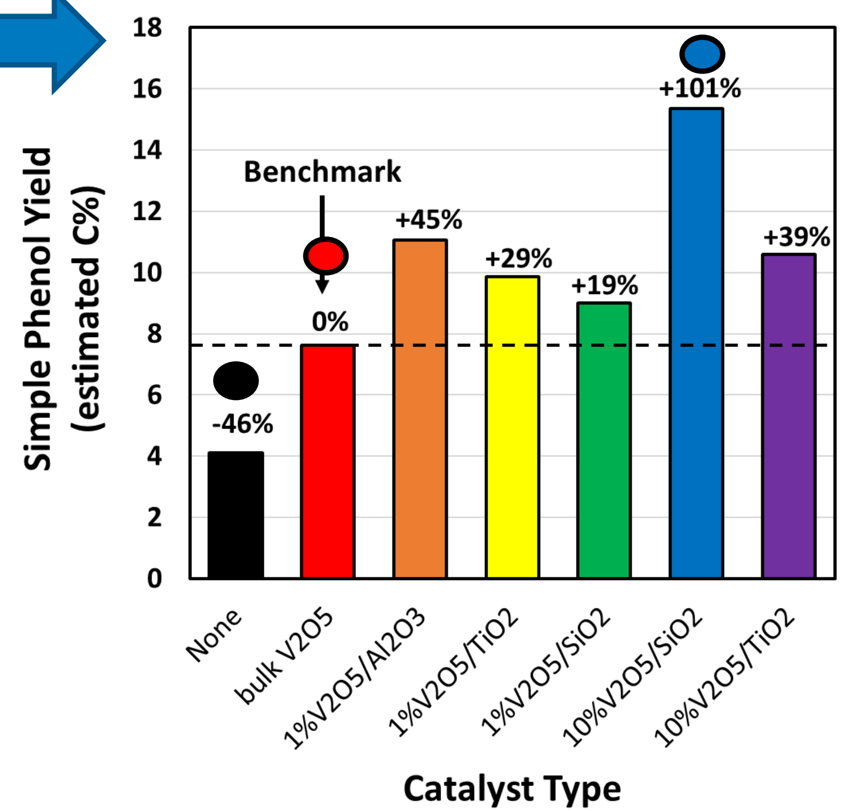


4. Progress / Accomplishments (5a of 8)

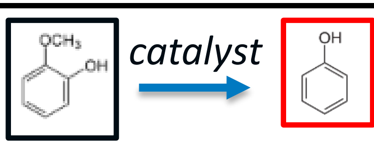
5. Reaction Testing with Whole Vapors and Model Compounds: 2x improvement in simple phenol yields from DMR lignin as compared to commercial catalyst.

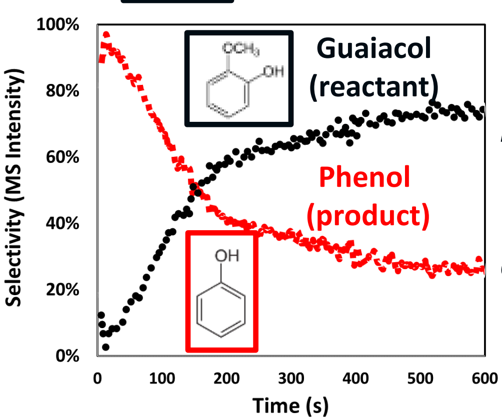
Improvements in simple phenol yields	
● 4%	**Uncatalyzed (pyrolysis-only)**
● 8%	**Benchmark catalyst**
● 15%	**NREL-developed catalyst** *(25% based on lignin content of DMR-EH residue)*

Phenol yields from whole vapors from DMR lignin pyrolysis



Experiments consistent with computational predictions.





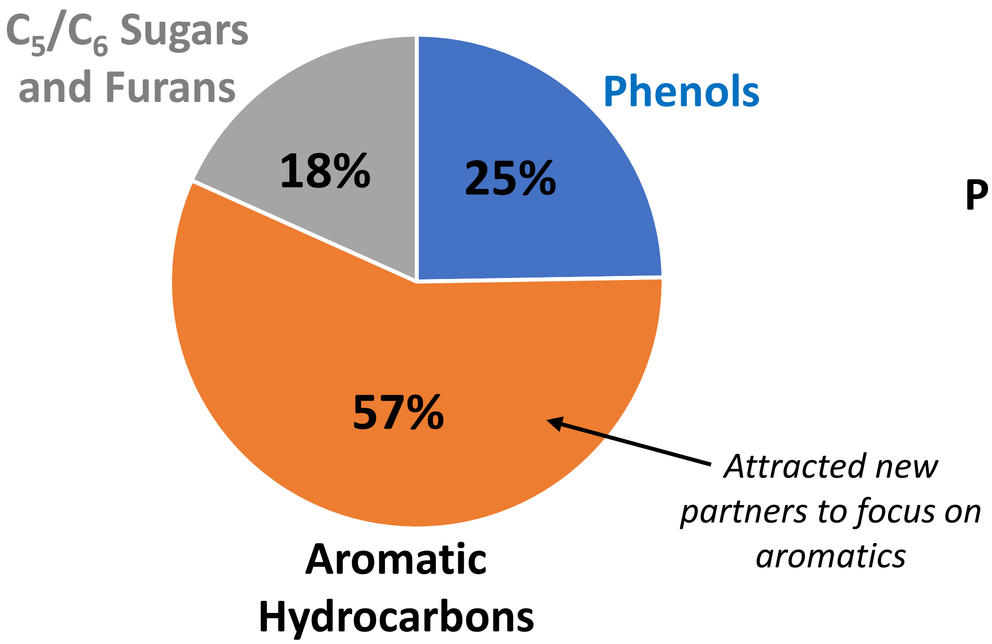
Model compound reaction experiments in good agreement with computational predictions

Guaiacol over NREL catalyst on TiO_2 at 450°C.

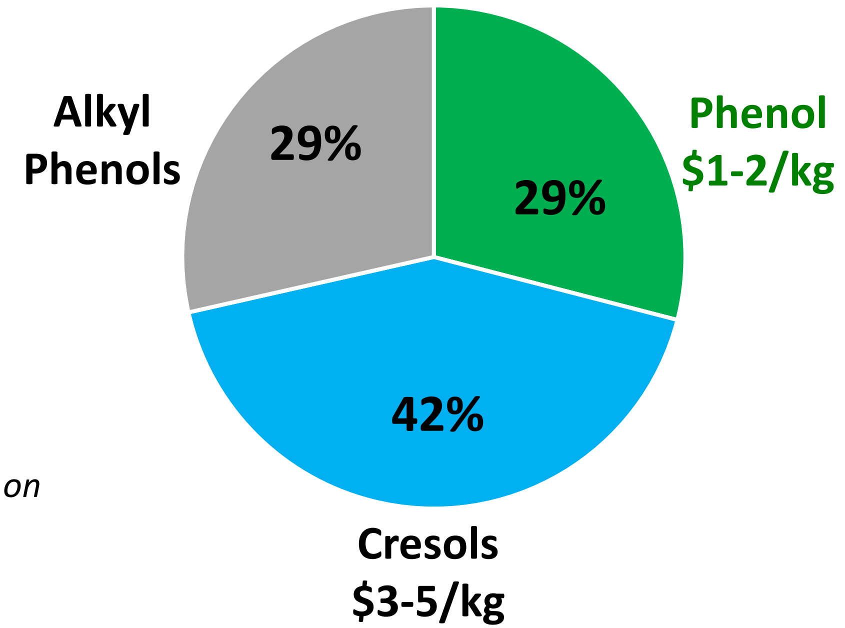
4. Progress / Accomplishments (5b of 8)

5. Reaction Testing with Whole Vapors: Condensed Product Composition

Compositions of Condensed Liquid Product



Distribution of Condensed Phenolic Compounds



Opportunity to increase phenolic yield by reducing aromatics (catalyst activity)

Opportunity to improve revenue by making higher value phenolics (cresols)

Conditions: 1:1 lignin to catalyst ratio, VOx/TiO2 catalyst at 550°C into dry ice condenser; analysis by GC/MS

4. Progress / Accomplishments (6 of 8)

6 & 7. Establish TEA impact, iterate, and improve: Process modifications and iterations in catalyst design have shown additional opportunities to improve phenol yield.

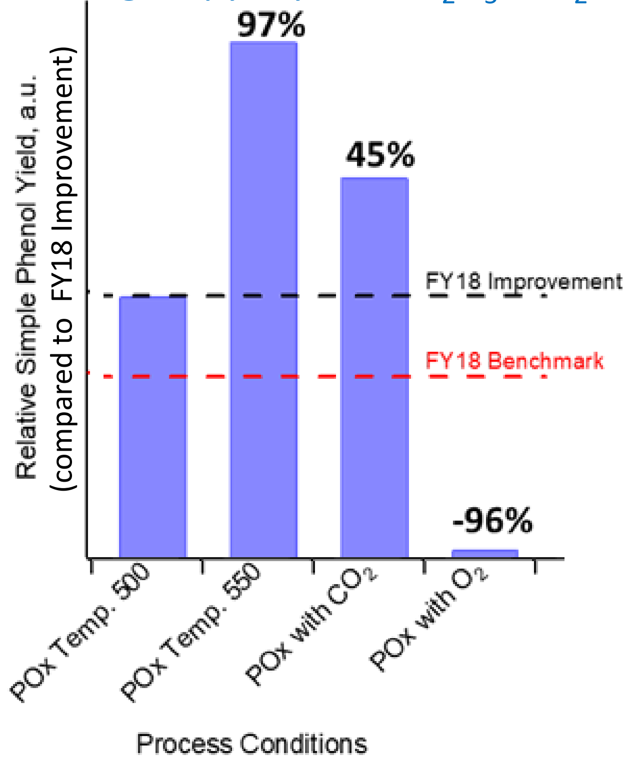
TEA Impact Correlated with Phenol Yield:

Relevant Criteria	Benchmark	Status	Future Target
Lignin conversion to phenolics	8%	**15%**	>25% (10% FY20)
Estimated TEA impact on MFSP reduction	$0.25/GGE	**$0.60/GGE**	>$1.35/GGE

Iterative R&D is assessing the impacts of pyrolysis/catalysis temperatures and oxidant co-feed and have shown significant impact on phenol yields. 2nd-generation catalysts have lowered vanadia loading and achieve dispersed active sites.

Varying Process Parameters (temperatures and oxidant co-feed)

Phenolic yields from whole vapors from DMR lignin pyrolysis on V_2O_5/TiO_2



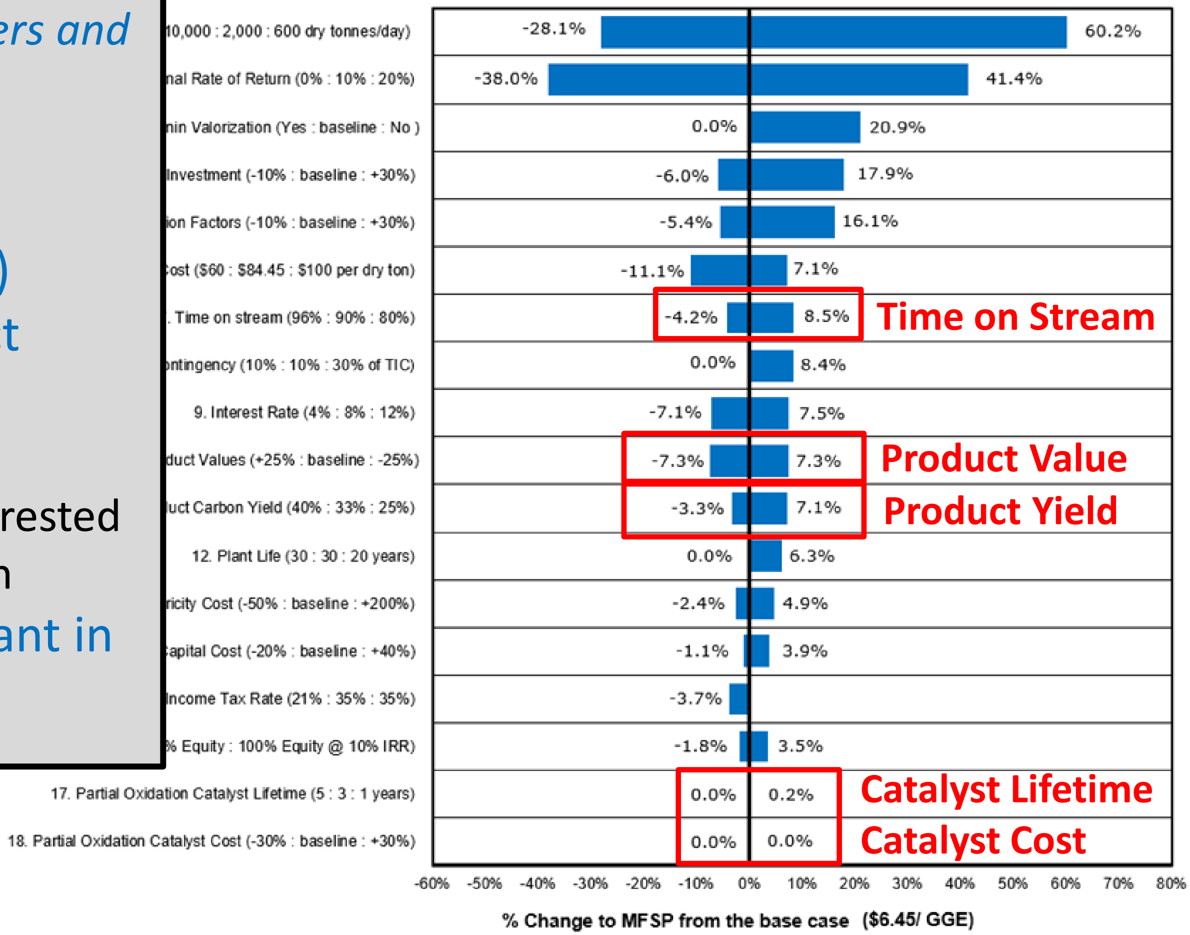
6 & 7. Establish TEA impact, iterate, and improve: Process modifications and iterations in catalyst design have shown additional opportunities to improve phenol yield.

Use TEA to inform research

Determine important cost-drivers and direct research towards those activities

- Time on stream (uptime)
- Carbon yield and product value
  - Valorize aromatics
  - Pursuing partners interested in aromatic production
- Catalyst cost is insignificant in overall process

Sensitivity Analysis ("Tornado Plot"): Emphasis on Yield



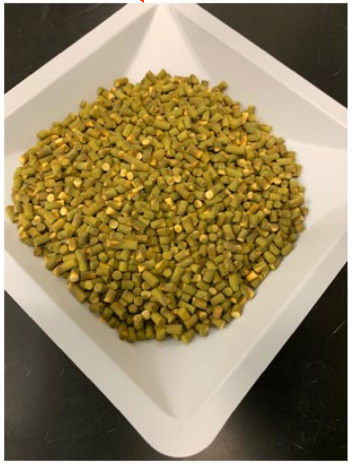
3. Progress / Accomplishments: Scale-up (8a of 8)

8. Scale-up and reduce uncertainty: Process modifications and iterations in catalyst design have shown additional opportunities to improve phenol yield.

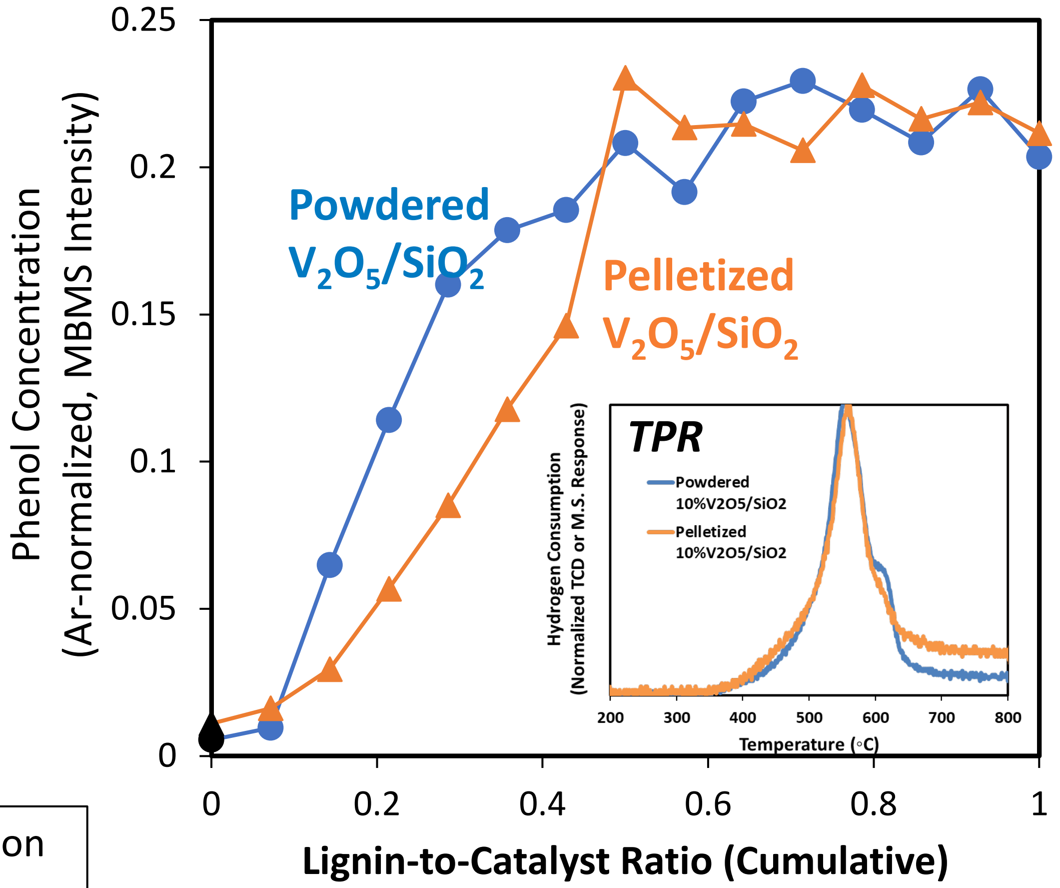
2 g powdered V_2O_5/SiO_2

100x larger batch prep.

200 g pelletized V_2O_5/SiO_2



Synthesis of technical catalyst: Wet impregnation of SiO_2 with vanadium oxalate + oxalic acid aqueous solution.



M.M. Yung et al., in prep.

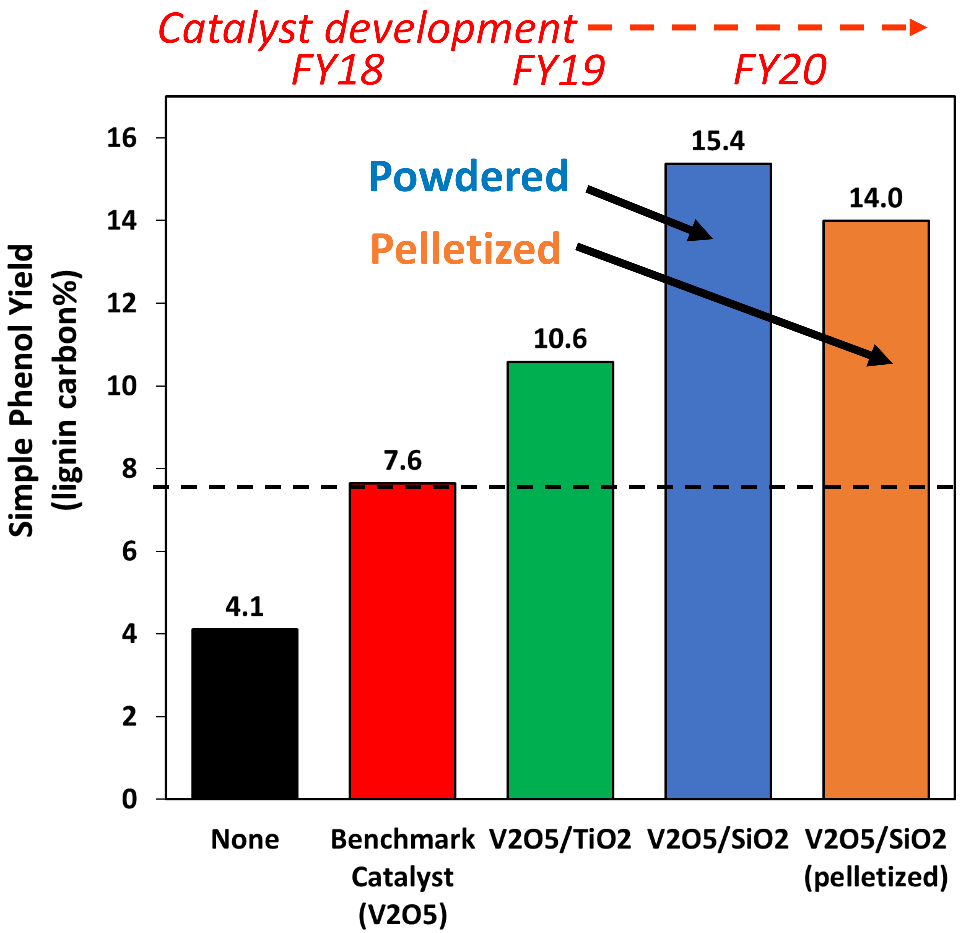
DMR-EH Lignin

Outcomes:

- 2x increase over benchmark yield to phenols
- 100x increase in catalyst batch size (>90% performance)
- 10x increase in test (500 mg to 5000 mg)

Technical Catalyst

Condensed Phenolics



1. Overview
2. Approach - Technical
3. Management
4. Progress and Accomplishments
5. Impact

5. Impact

5. Impact - Addressing BETO Barriers and Goals (1 of 3)

Project Outcomes and Relevance – Reduce biofuel production cost by valorizing lignin via gas phase selective oxidation to make phenolics

- Focus on products with large markets, high value, and potential for bio-adoption
- Novel approach provides portfolio diversification and low-cost route

BETO MYP Barriers

Ct-C. Process Development for Conversion of Lignin
Ct-F. Increasing the Yield from Catalytic Processes
Ct-K. Developing Methods for Bioproduct Production
Ot-B. Cost of Production

- Developing catalysts for gas phase oxidation to produce high yields of valuable phenols from low-value lignin will reduce biofuel production

Relevant Criteria	Benchmark	Status	Long-Term Target
Lignin conversion to phenolics	8%	15%	>25%
Estimated TEA impact	$0.25/GGE reduction	$0.60/GGE reduction	>$1.35/GGE reduction

BETO Performance Goals (New BETO MYP):

By 2030, verify hydrocarbon biofuel technologies that achieve ≥50% reduction in emissions relative to petroleum-derived fuels at **$2.5/GGE MFSP**

↓

- Providing ***early-stage R&D*** to enable verification reduce risk
- ***Identifying viable routes to $2.5/GGE*** through phenolic co-products, combing catalyst and process development

5. Impact – Addressing Bioenergy Industry (2 of 3)

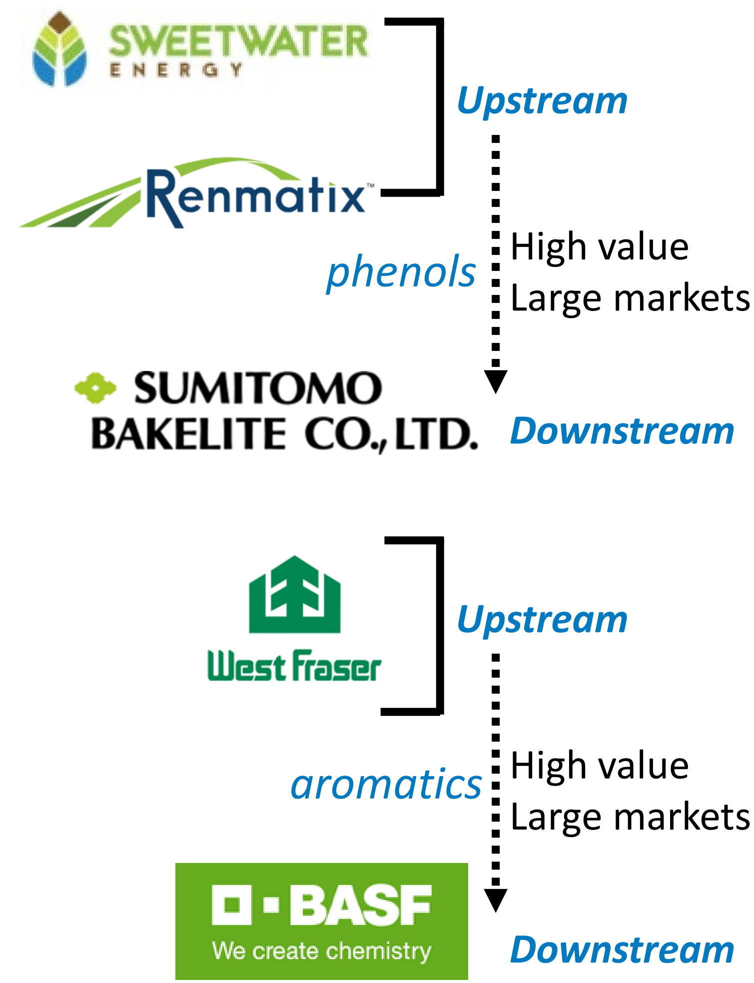
Industrially-relevant for both established and emerging companies in providing routes to renewably-sourced products to penetrate existing markets and develop new markets.

- Interest from both ***upstream and downstream*** companies (lignin producing biorefineries and phenol consumers)

- **Technology applies to a variety of processes and lignin sources/types**

- ***Market demand*** from existing companies to use renewably-sourced precursors for production of polycarbonates and plastics
  - Create a **cost-competitive** technology for bio-phenol production
  - Focus on products with large markets, high value, and potential for bio-adoption
  - **Market size could support >200 biorefineries**

- Creates a ***diversified revenue stream***



5. Impact – Science and Partnerships (3 of 3)

Developing Foundational Science and Generating Intellectual Property

Record-of-Invention and Patent Application (1)

External Presentations (16)

Publications (2*)

*Submission following patent issuance.

Building Industrial Partnerships

Lignin-to-Phenols

SWEETWATER ENERGY

Renmatix

SUMITOMO BAKELITE CO., LTD.

JM Johnson Matthey Inspiring science, enhancing life

Lignin-to-Aromatics

BASF We create chemistry

West Fraser

Training and Support for Next-Generation Engineers/Scientists

7 Undergraduate Internships and
2 Post-doctoral Researchers Supported

Summary

Goal: Develop catalysts and process to convert lignin pyrolysis vapors into valuable phenols, adding a diversified revenue stream to enable economic biofuels

-Project target: 10% yield to phenolics by 2020 on bench-scale

-Status: 15% yield to phenolics on lab-scale *($0.60/GGE MFSP reduction)*

-Future Target: 30% yield to phenolics + aromatics with industrial (pulp) lignin

1) Approach:

- Integrated, collaborative approach to catalyst design for selective oxidation of lignin to produce valuable phenolics
- Develop catalytic materials by varying **bond strength and site density**

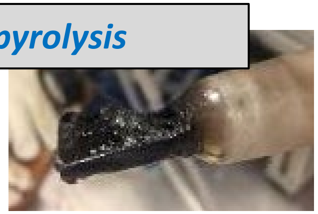
2) Impact and Relevance to BETO & Industry

- Address critical challenges (adding value from lignin and improve yield of catalytic processes)
- Focus on BETO barriers and performance targets
- **Renewable, cost-competitive phenols are of interest to industrial partners (upstream and downstream) – diversify revenue streams**

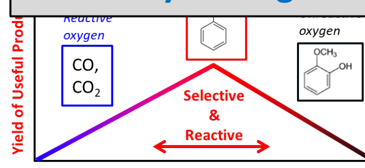
3) Technical accomplishments:

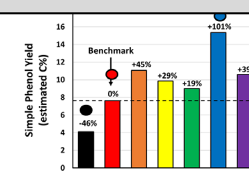
- Developed catalysts with 2x improvement in phenol yield over commercial benchmark catalyst
- 10x scale-up in reaction size
- 100x in catalyst batch size
  - Bench-scale testing not performed
- Successful regeneration of catalysts
- Economic sensitivity analysis
  - Estimated MFSP reduction of $0.60/GGE

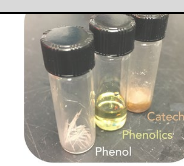
Lignin pyrolysis



Catalyst design to achieve high phenol yields and $$$







Acknowledgments

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- Kayla Brady
- Eric Romero
- Matt Kastelic
- Fatima Zara
- Jon Wells
- Kylie Smith
- Marissa Leshnov

U.S. DEPARTMENT OF ENERGY

BETO Consortia Partners

ChemCatBio Chemical Catalysis for Bioenergy

CCPC

www.cpcbiomass.org

Industrial Partners

SWEETWATER ENERGY

Renmatix

BASF We create chemistry

West Fraser

NREL Biomass Catalysis & Reaction Engineering Group

Summary

Goal: Develop catalysts and process to convert lignin pyrolysis vapors into valuable phenols, adding a diversified revenue stream to enable economic biofuels

-Target: 30% yield to phenolics + aromatics with industrial (pulp) lignin by 2021

***-Status: 15% yield to phenolics on lab-scale** ($0.60/GGE MFSP reduction)*

1) Approach:

- Integrated, collaborative approach to catalyst design for selective oxidation of lignin to produce valuable phenolics
- Develop catalytic materials by varying **bond strength and site density**

2) Technical accomplishments:

- Developed catalysts with 2x improvement in phenol yield over commercial benchmark catalyst
- **Estimated MFSP reduction of $0.60/GGE since 2017**

3) Relevance to Bioenergy Industry

-Address critical challenges (adding value from lignin and improve yield of catalytic processes)

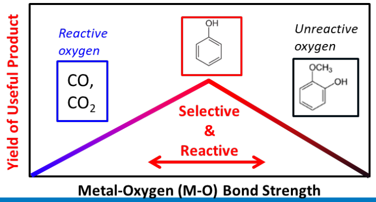
-Focus on BETO barriers and performance targets

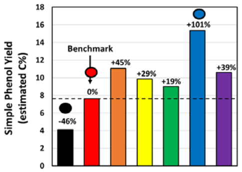
-Renewable, cost-competitive phenols and aromatics are of interest to industrial partners (upstream and downstream) – diversify revenue streams

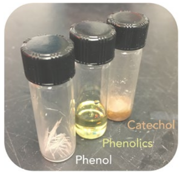
4) Future work:

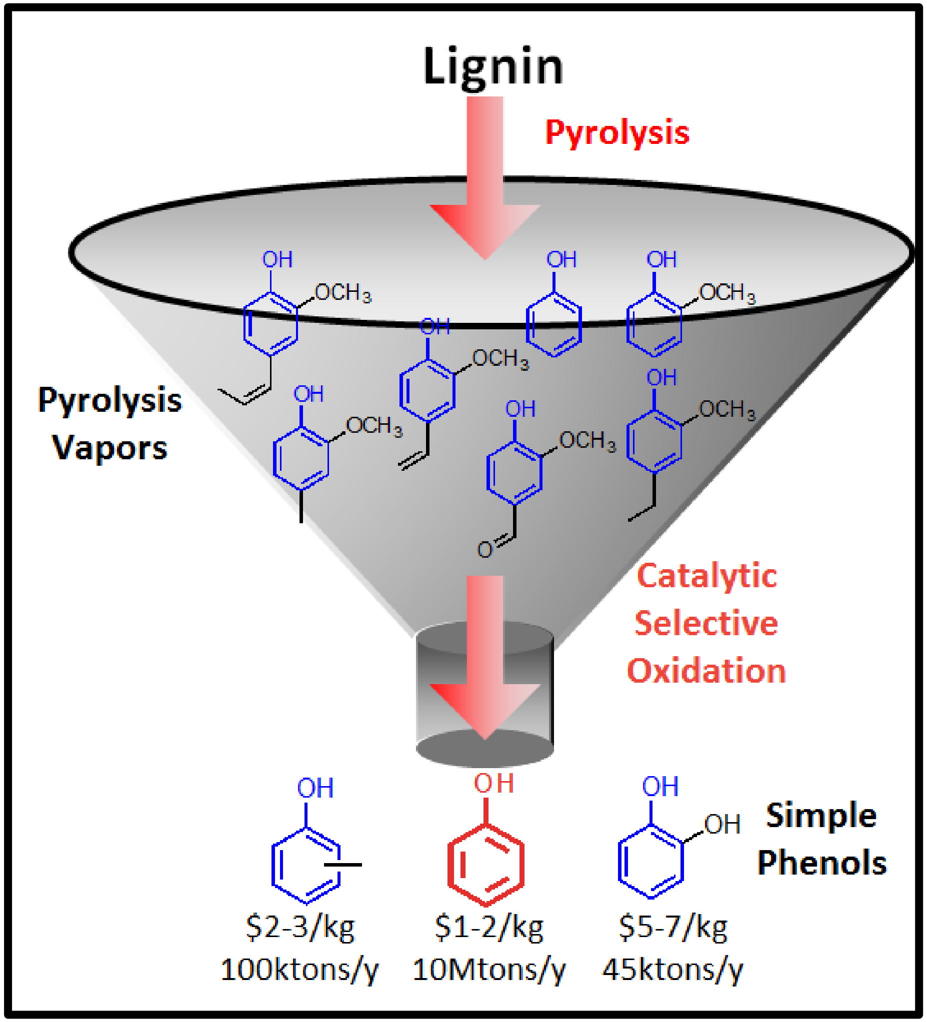
- Improve **yields** (phenol + aromatics)
- Utilize **feedstock** from industrial partners
- **Scale-up** catalyst and lignin feeding for **bench-scale demonstration**

Lignin pyrolysis ⟷ Catalyst design to achieve high phenol yields and $$$





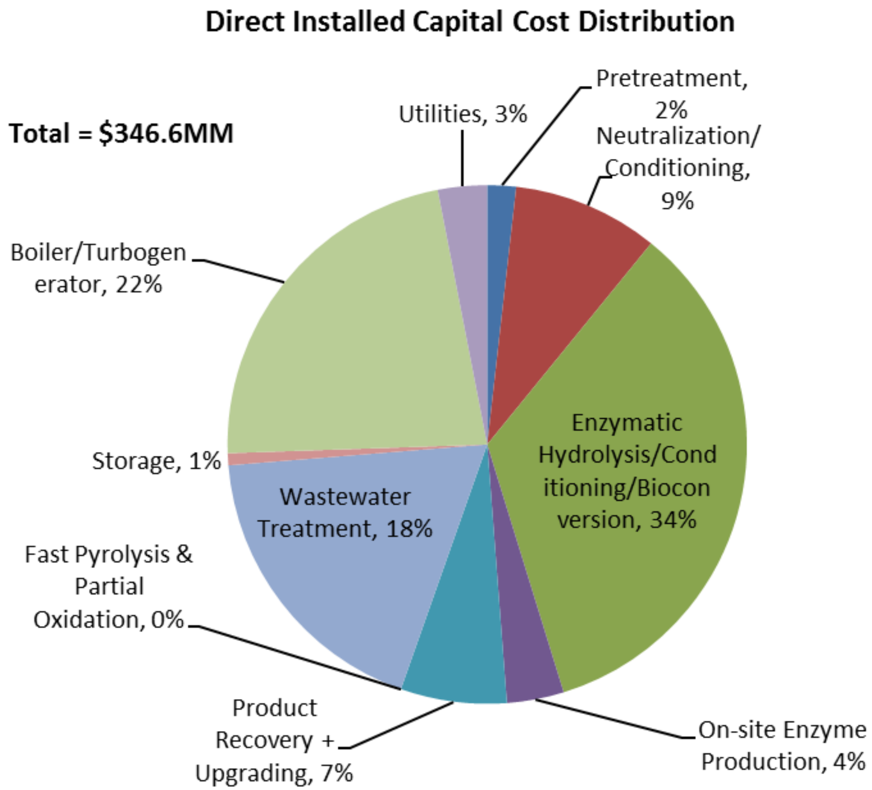


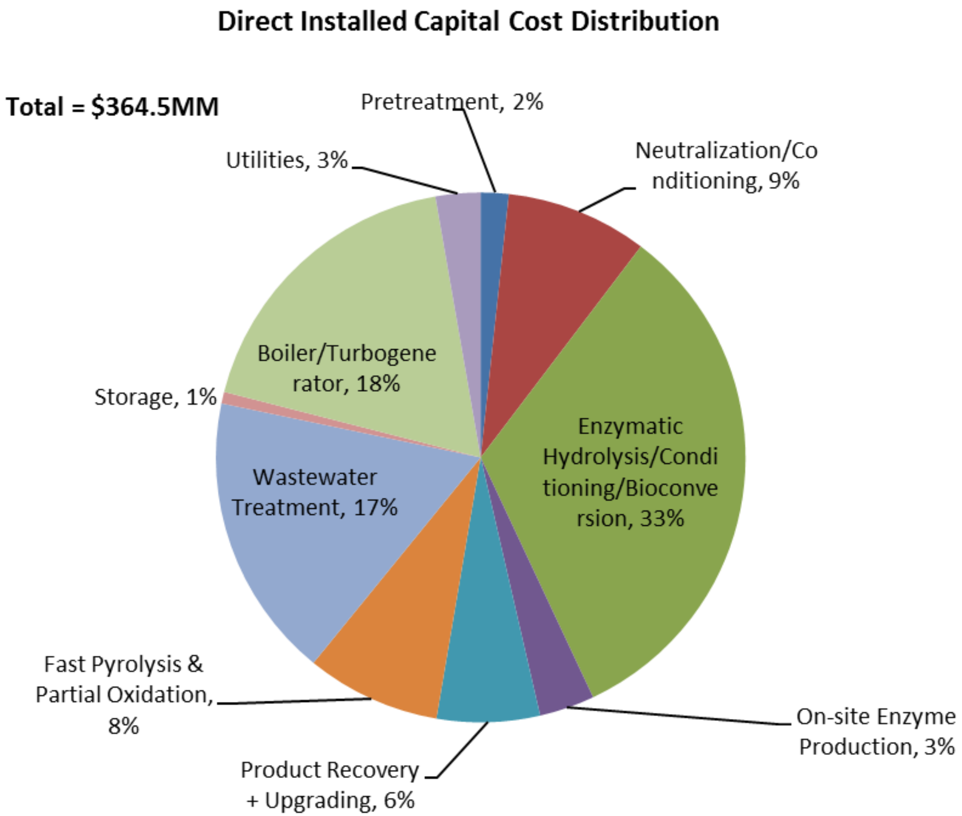

Lignin
Pyrolysis
Pyrolysis Vapors
OH
OCH3
Catalytic Selective Oxidation
Simple Phenols
$2-3/kg
100ktons/y
$1-2/kg
10Mtons/y
$5-7/kg
45ktons/y

TEA: Capital Cost Breakout

Lignin to Heat & Power (no coproduct)

Lignin Valorization (Coproduct: phenols)





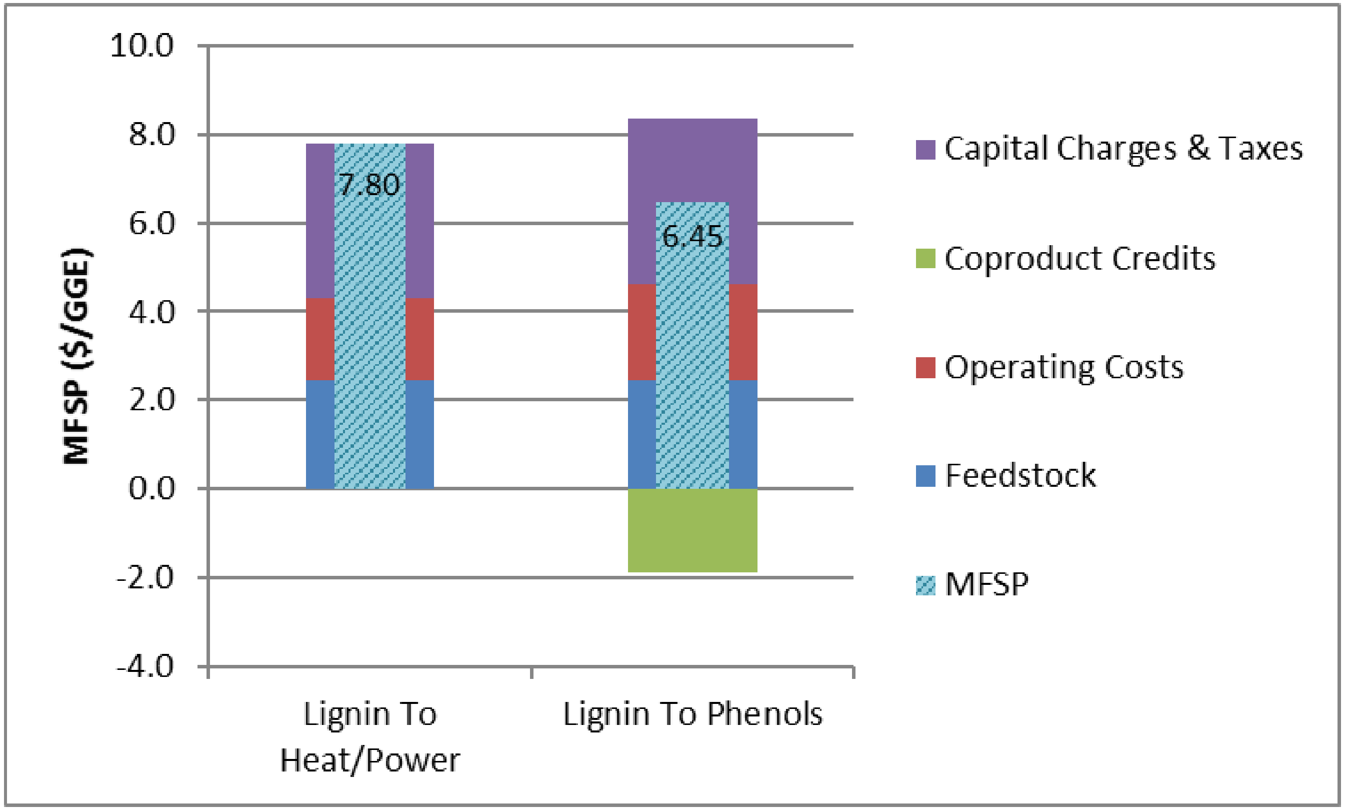
Costs in 2014$

TEA Results

17% MFSP improvement from valorization of lignin

Costs in 2014$

Phenols coproduct value: $1,981/tonne (2010-2014 5-yr average from IHS)



Note: The $7.80/GGE MFSP number for the pathway (via lipids) was presented in the DOE Bioenergy Technologies Office (BETO) Project Peer Review (Denver, CO) (https://www.energy.gov/sites/prod/files/2017/05/f34/Biochemical%20Platform%20Analysis%20Project_0.pdf, see slide 11).

Mass Flow

100 g of DMR-EH reside
(60 g lignin and 40 g other/residual sugars)

Solid (char, coke) (30 g)

Liquid (60 g)

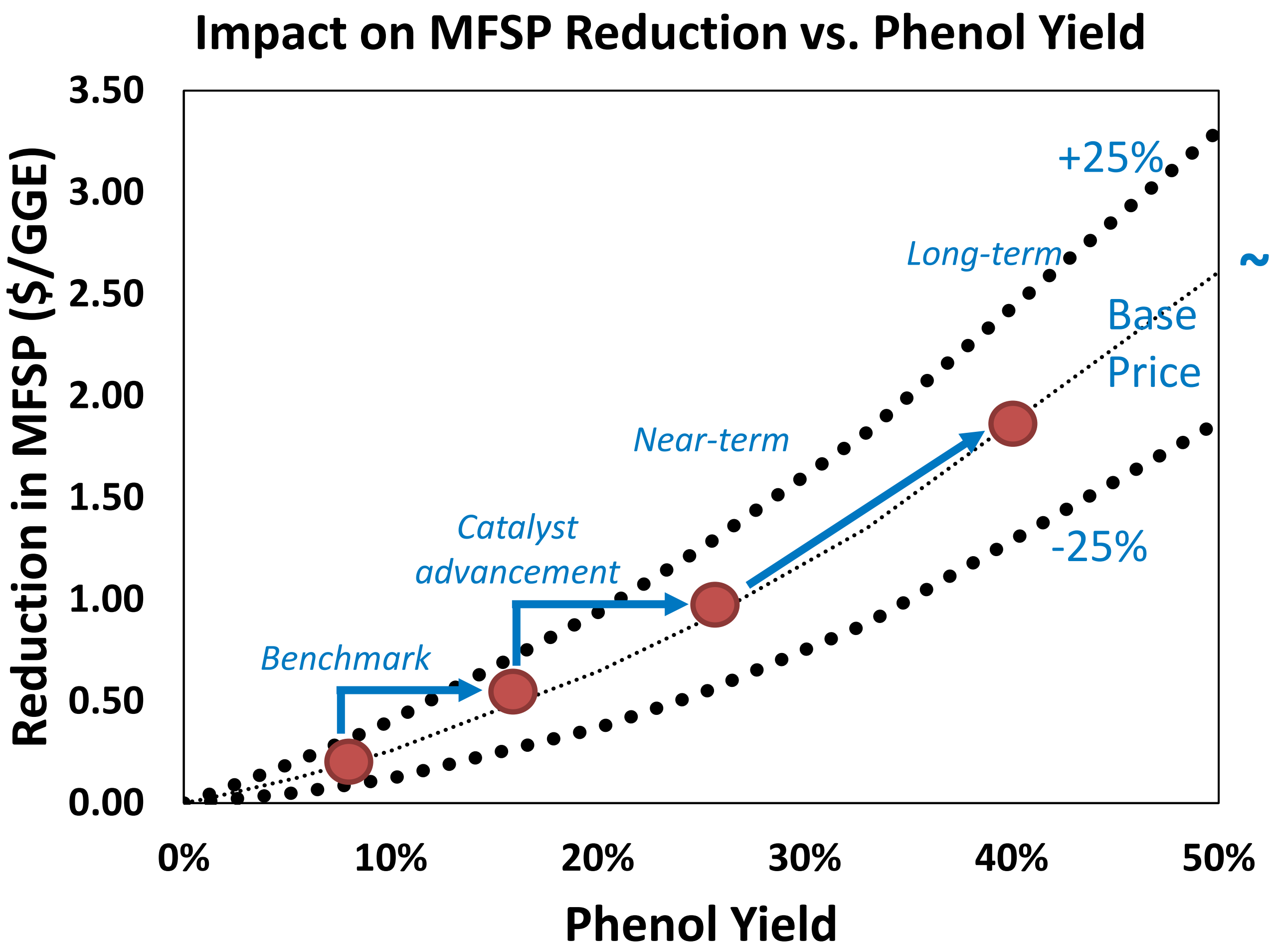
Gas (H_2O, CH_4, CO, CO_2) (10 g)

32 g Aromatic hydrocarbons

15 g Simple phenols

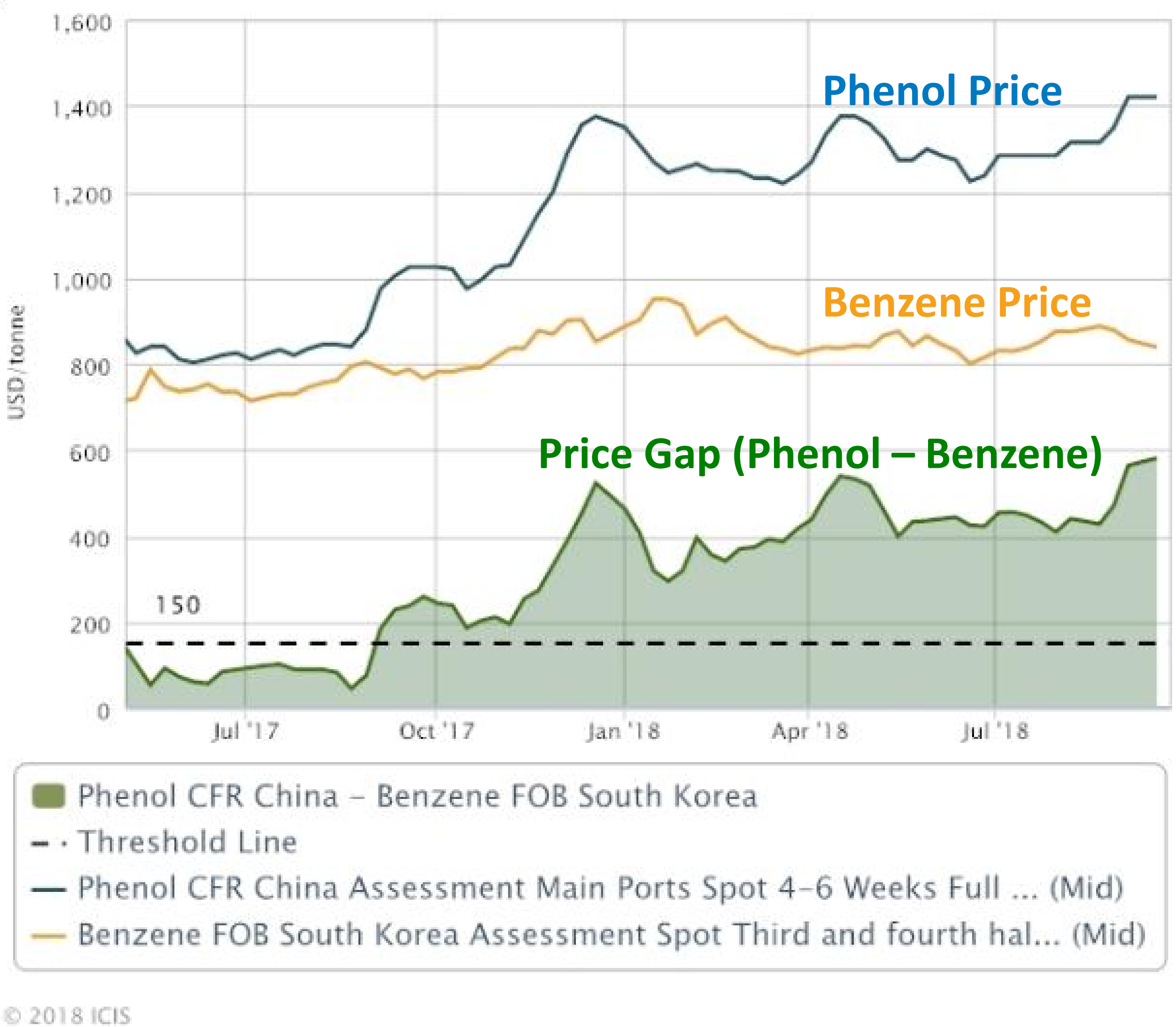
13 g C5/C6 sugars and furans and others

Outcomes from technology advancements



~$0.80/lb

Phenol value and price gap relative to benzene



~$0.60/lb

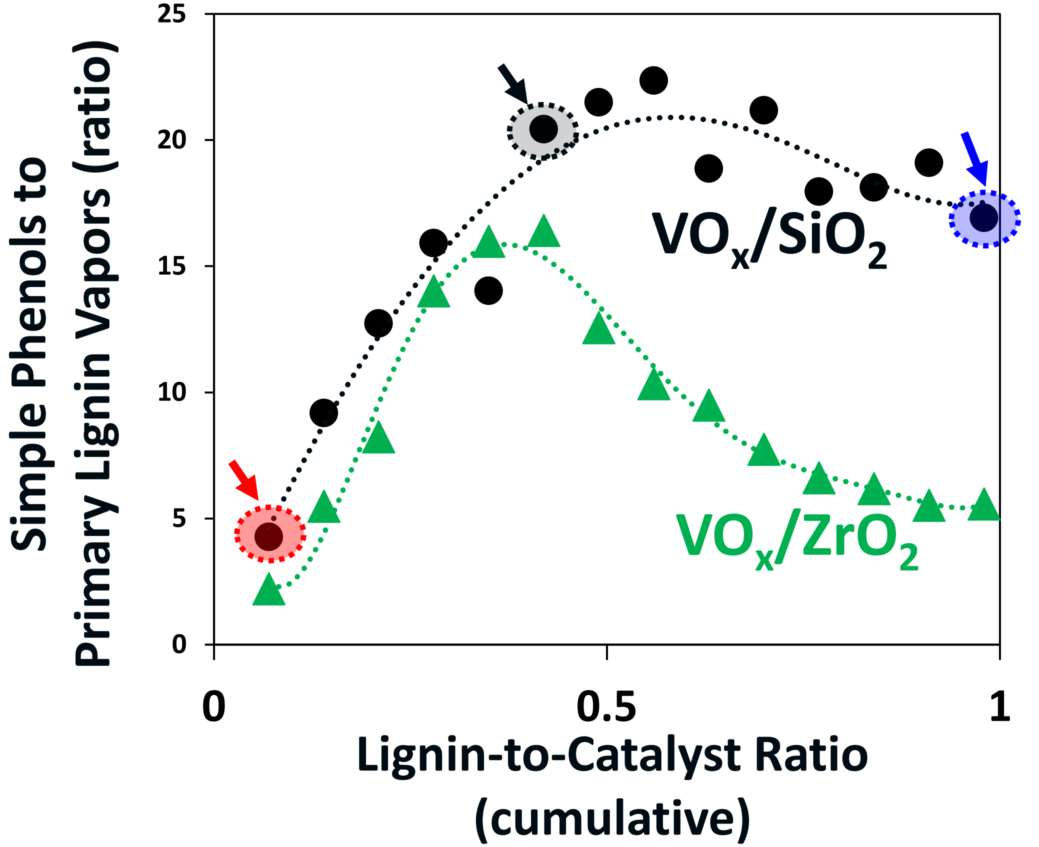
Higher incentive for integrated phenol producers to produce phenol instead of selling benzene

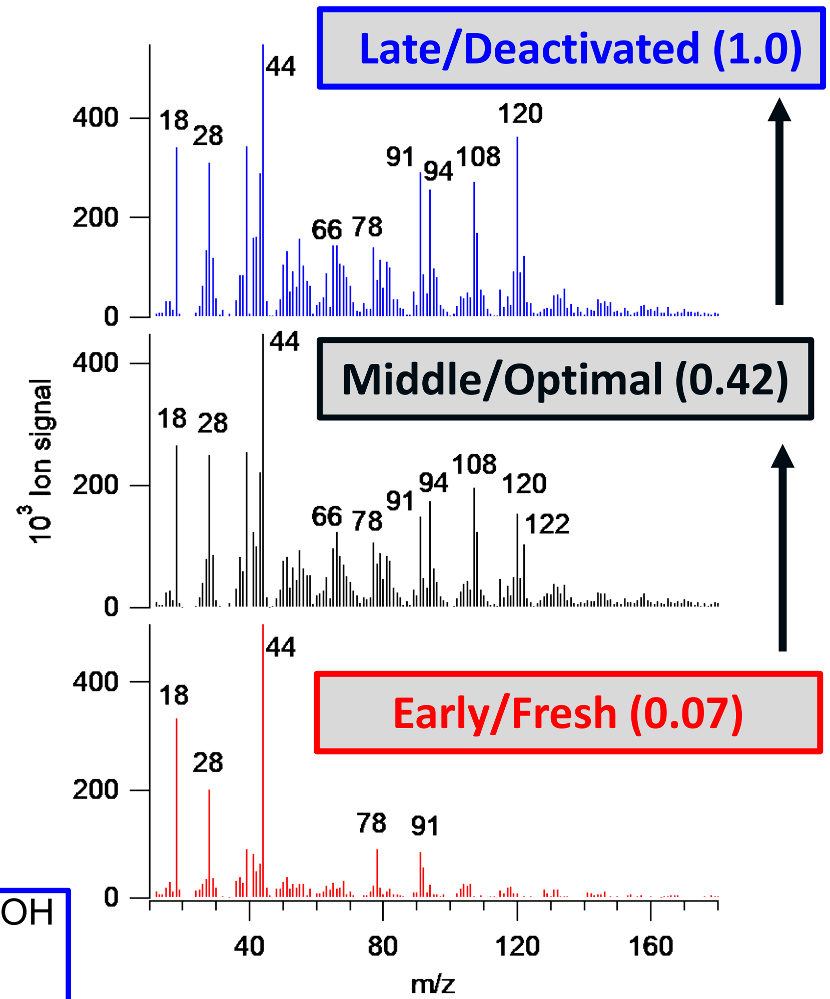
Lower incentive for integrated phenol producers to produce phenol instead of selling benzene

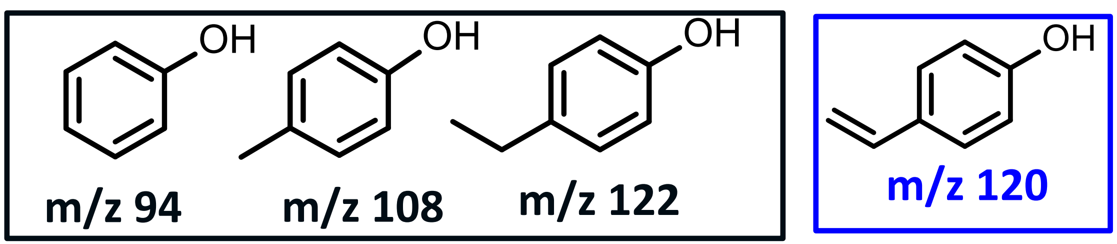
https://www.icis.com/explore/resources/news/2018/09/26/10261917/china-phenol-import-prices-at-near-4-year-high-on-tight-supply/

Reactivity affected by composition and exposure time

Product yield and distribution change with type of catalyst and time on stream

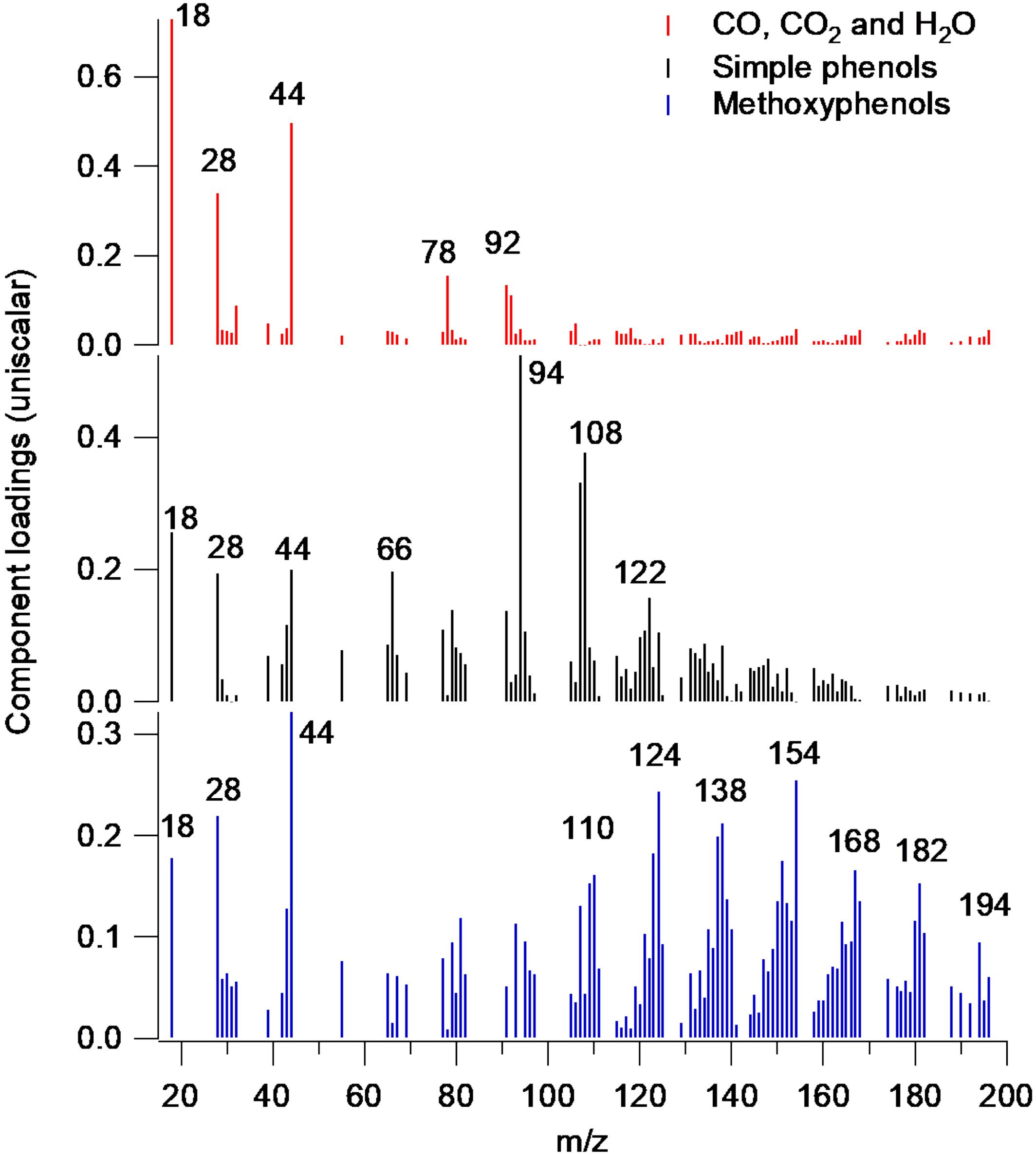






*MBMS spectra from 5%V_2O_5/SiO_2

Multivariant analysis of MBMS data



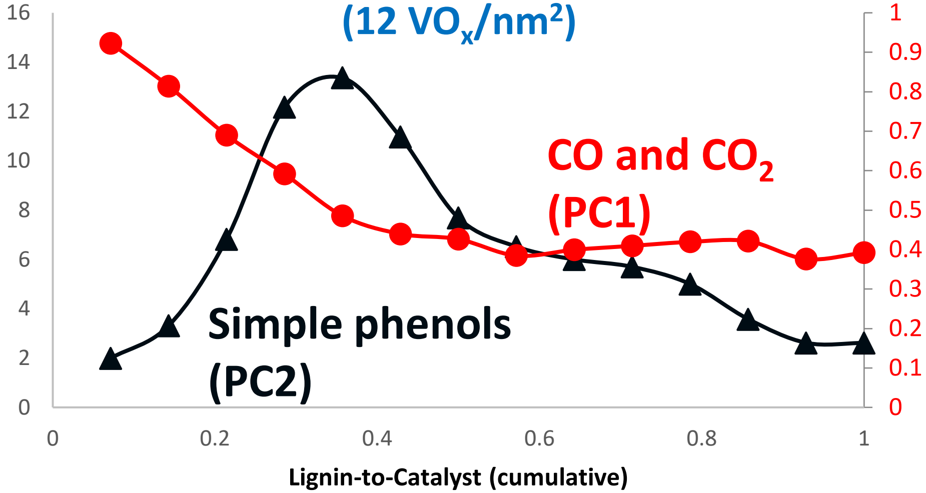
Mass spectrum 1: (PC1)
CO, CO_2 and H_2O, plus some aromatics

Mass spectrum 2: (PC2)
Simple phenols (desirable products)

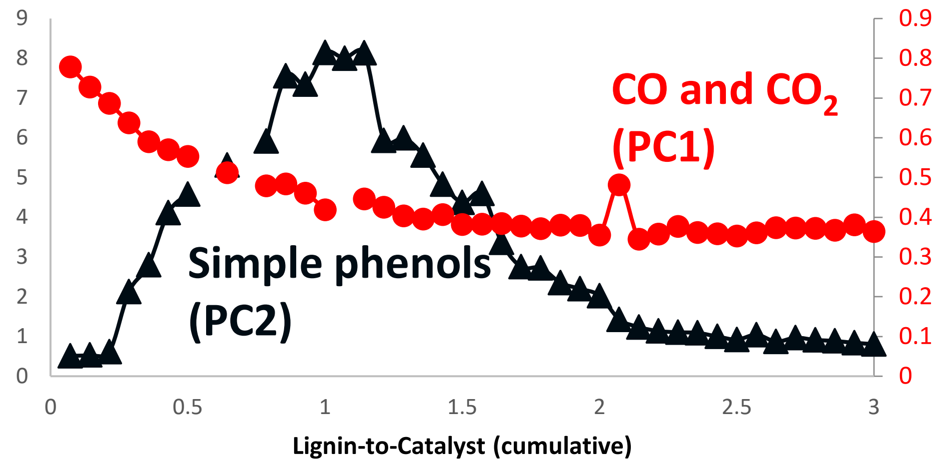
Mass spectrum 3: (PC3)
Methoxy phenol (direct lignin pyrolysis) – “breakthrough products”

Partially reduced surface improves partial oxidation

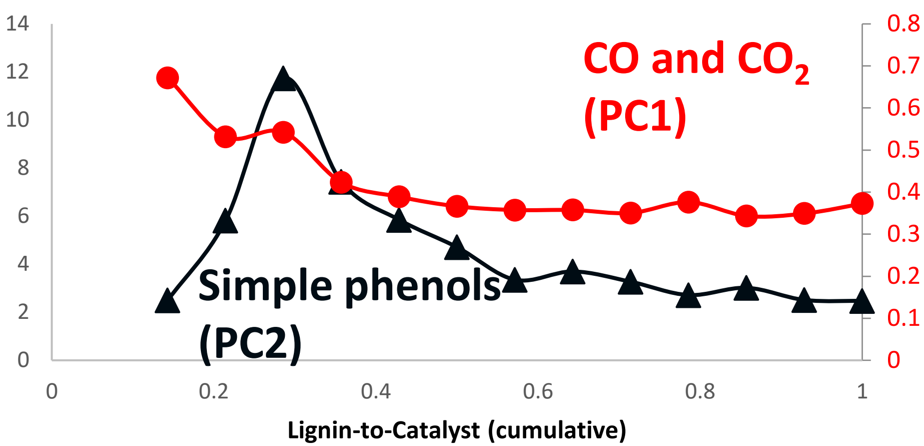
$10\%V_2O_5/ZrO_2$ (12 VO_x/nm^2)



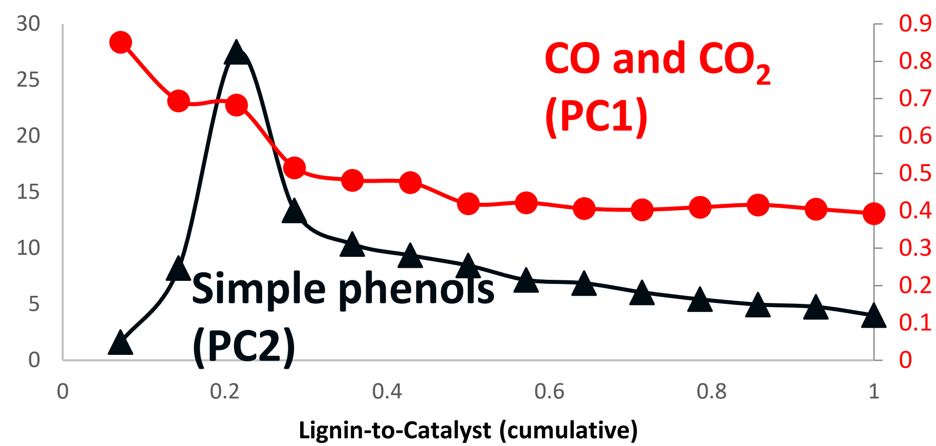
$10\%V_2O_5/SiO_2$ (Sweetwater Ultra) (5.1 VO_x/nm^2)



$1\%V_2O_5/SiO_2$ (0.5 VO_x/nm^2)



$10\%V_2O_5/SiO_2$ (5.1 VO_x/nm^2)



Reactivity affected by composition and exposure time

Phenol yield during lignin pyrolysis