Renewable Fuel Additives from Woody Biomass

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DOE Bioenergy Technologies Office (BETO)
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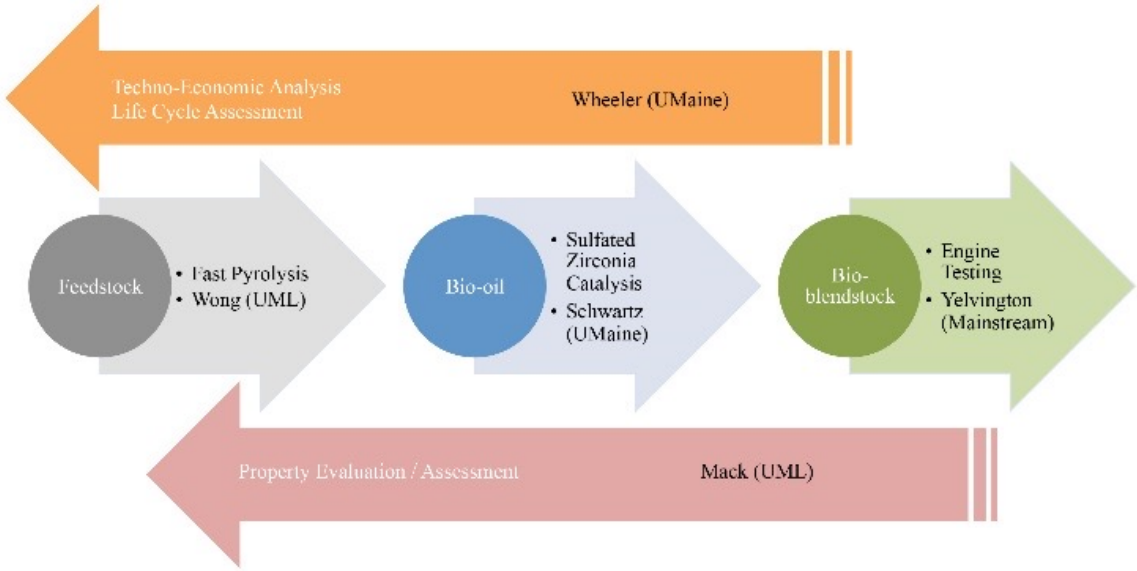
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

BIOENERGY TECHNOLOGIES OFFICE

Project Overview

Co-Optimization of Fuels & Engines

- The project team proposes an integrated approach to the development and production of ***bioblendstocks that improve the energy density, sooting propensity, and cetane number of base diesel fuel*** while maintaining cold weather behavior.
- The process converts sawmill residues into bio-oil through selective fast pyrolysis; the bio-oil is then selectively upgraded to form selectively oxygenated, minimally-branched hydrocarbons using non-noble metal catalysts in combination with metal-catalyzed hydrogenation.
- Advanced predictive models, in conjunction with existing property databases, and experimental testing are used to evaluate overall bioblendstock properties and their impact on base diesel fuel. An iterative, targeted upgrading approach is implemented to optimize the proposed bioblendstock's performance.
- Assessment includes a techno-economic analysis, a life-cycle assessment, and engine testing.



Successful identification of next-generation bio-derived fuels can boost fuel economy and vehicle performance while reducing emissions

The key challenge is to identify a fuel with the desired properties that can be economically produced with minimal environmental impact

Management

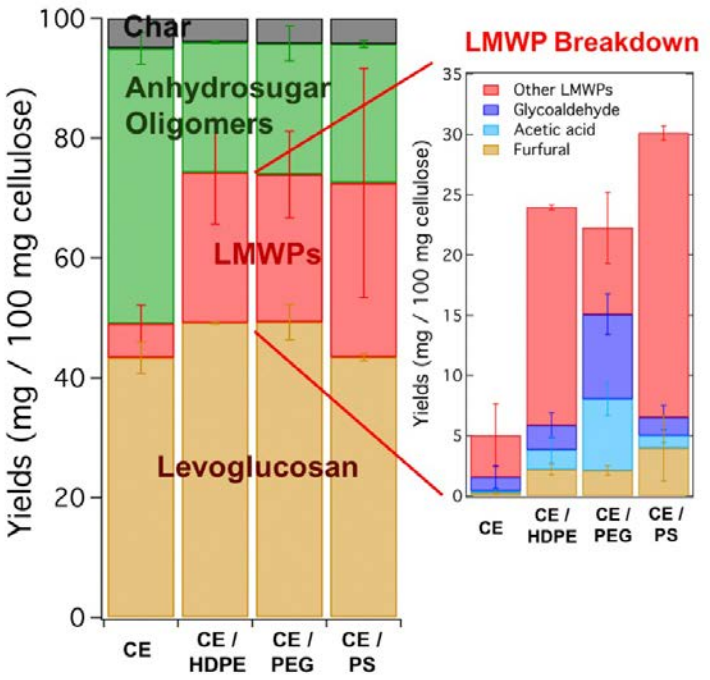
- This project is part of the **Co-Optimization of Fuels & Engines**, which involves 9 DOE National Laboratories, >20 universities, and industry partners. Coordination and collaboration activities include:
  - Participation and attendance at regular and annual project meetings
  - Data sharing and collaboration with other participants
  - Communication with National Lab Mentor (Dr. Daniel Gaspar, PNNL)
  - Monthly Co-Optima Teleconferences with industry stakeholders and project leadership
- **Project Structure**
  - Property Predictions & Fuel Evaluation – Hunter Mack (University of Massachusetts Lowell)
  - Fast Pyrolysis & Bio-oil Production – Hsi-Wu Wong (University of Massachusetts Lowell)
  - Catalytic Upgrading – Thomas Schwartz (University of Maine)
  - Technoeconomic Analysis & Life Cycle Assessment - Clayton Wheeler (University of Maine)
  - Engine Testing – Michael Cutbirth (Mainstream Engineering)
- **Project management** is led by the principal investigator (Mack) with input from DOE BETO and Co-Optima
- **Risk identification and mitigation** is managed through close collaboration of the principal investigators, multiple feedback loops during process development, and oversight/direction from DOE BETO and the Co-Optima team

Approach

Co-Optimization of Fuels & Engines

Selective Conversion of Biomass into Bio-oil by Fast Pyrolysis

- Lignocellulosic biomass has been recognized as a possible replacement for fossil-derived resources to produce drop-in fuels.
- Fast pyrolysis is a promising technology to convert biomass into fuels with the potential to be 2 to 3 times less expensive than other competing approaches, such as fermentation and gasification.
- The main obstacle is to gain precise control of the compositions and properties of the resultant bio-oil, since a wide array of biomass feedstocks with different fractions of cellulose, hemicellulose, lignin, and additives (such as minerals and salts) exist.
- The bio-oil produced directly from fast pyrolysis also contains high degree of oxygen, causing issues of high acidity, low heating value, high viscosity, and poor chemical stability.
- This project aims to unravel the parametric effects of feedstock properties and reaction operation conditions on bio-oil and individual products yields for pine sawdust pyrolysis to obtain optimal bio-oil compositions that can be either directly used as part of next-generation bio-blendstocks or easily upgraded with advanced catalysis strategies.



- Task 1.1.1 (Identify optimal mixing patterns and biomass feedstocks for fast pyrolysis)
- Task 2.1.1 (Derive parametric expression of bio-oil compositions)
- Task 3.2.1 (Production of bio-oil using a bench-scale fluidized bed pyrolysis reactor)

Approach

Co-Optimization of Fuels & Engines

Catalytic Upgrading

- The principal challenge associated with the use of bio-oils as fuels or fuel additives is the high oxygen content, coupled with the high acidity of certain oxygenates present in most bio-oils.
- We use a **novel** combination of selective pyrolysis via micro-mixing manipulation and chemical catalysis to tune the final properties of our bioblendstocks.
- In particular, we will focus on the application of sulfated zirconia and zeolitic catalysts to couple small-molecule organics and phenolics, thereby improving the energy density of the bio-oil and decreasing its acidity.
- The objective of this task is to show that a blendstock for diesel fuel can be produced in a tunable fashion by coupling furans with phenolics, both obtained from bio-oil.
- The furans and phenolics are first etherified to perform partial deoxygenation and chain elongation. The ethers are then hydrogenated to yield moderately branched oxygenates that can be effectively used as a blendstock for diesel fuel.

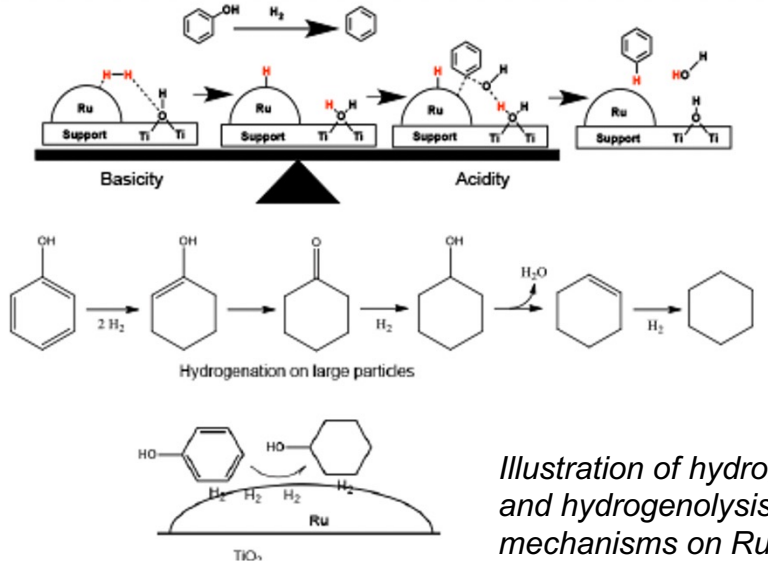


Illustration of hydrogenation and hydrogenolysis mechanisms on Ru/TiO_2 catalysts

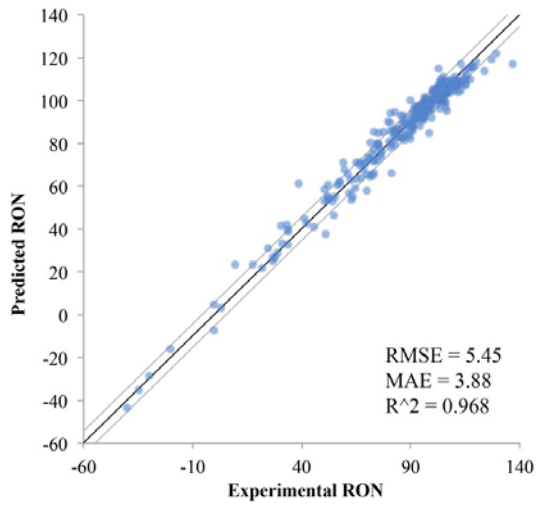
- Task 1.1.2 (Demonstrate production of etherified aromatics from bio-oil model compounds)
- Task 2.1.2 (Hydrogenation of etherified aromatics)
- Task 3.2.2 (Catalytic conversion using real bio-oil feedstocks)

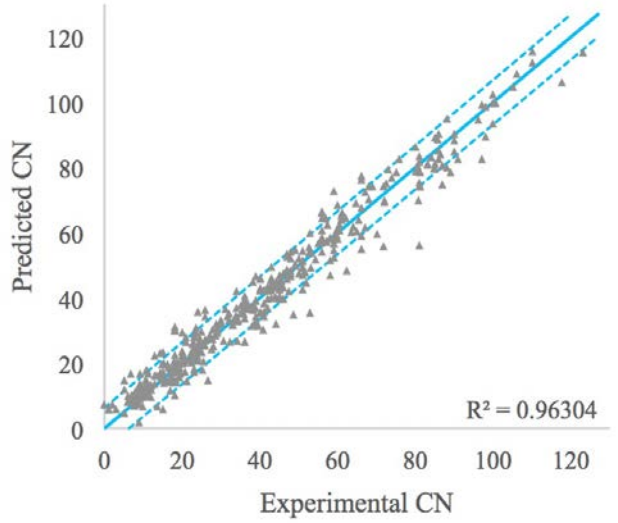
Approach

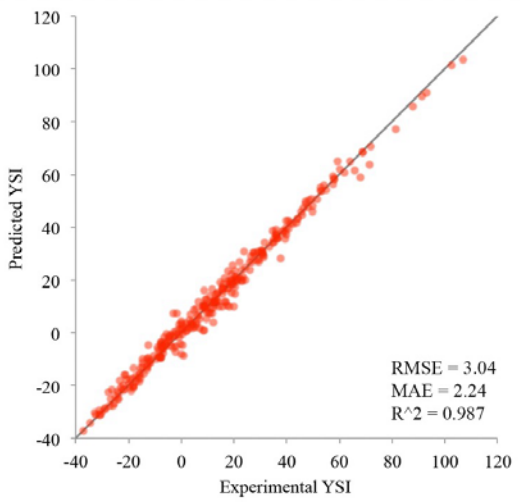
Co-Optimization of Fuels & Engines

Property Evaluation & Feedback

- In combination with existing experimental databases, predictive models have accelerated the development of new alternative fuels by shortening the feedback loop inherent to fuel research.
- Models, based on artificial neural networks, will be used to guide the proposed conversion process outlined above.
- The resultant bioblendstock will undergo a full composition analysis in concert with ASTM D975 (Standard Specification for Diesel Fuel Oils).
- Additionally, the impact of the bio-derived blendstock on energy density, sooting propensity, cetane number, and cold weather behavior (e.g. cloud point, pour point) will be assessed (in neat form and blended).







- Task 1.2.1 (Property Prediction Modeling)
- Task 2.2.1 (Bioblendstock Evaluation and Blending Models)
- Task 3.1.2 (Target Bioblendstock Analysis)

Approach

Co-Optimization of Fuels & Engines

Techno-economic Analysis & Life-Cycle Assessment

- UMaine's Forest Bioproducts Research Institute has developed a Multi-Criteria Decision Analysis (MCDA) Tool that integrates process techno-economic analysis (TEA), woody biomass feedstock logistics and life cycle assessment (LCA).
- The inputs include process-specific data from simulations to estimate product yields, green house gas emissions, heat, power, and water consumption along with emissions factors from the GREET model for input materials, biomass availability and harvesting models, and criteria selection to calculate cardinal scores for process alternatives.
- The current process will be simulated and integrated into the model to investigate the impacts of process alternatives based on the TEA and LCA results.

Sustainability Metrics for Fast Pyrolysis and Upgrading Conversion

Sustainability Metric	2009 SOT[1]	2012 SOT	2013 SOT	2014 SOT	2015 SOT	2017 Projected
Fossil GHGs (g CO_2-e/MJ fuel)	22.1	19.8	20.5	19.4	22.2	18.9
Fossil Energy Consumption (MJ fossil energy/MJ fuel)[2]	0.326	0.294	0.321	0.310	0.359	0.301
Total Fuel Yield (gal/dry ton wood; gge/dry ton wood)	74; 78	74; 78	84; 87	84; 87	83; 87	84; 87
Carbon-to-Fuel Efficiency (C in fuel/C in biomass)	38%	38%	47%	47%	48%	47%
Water Consumption (m^3/day; gal/GGE fuel)[3]	998; 1.5	998; 1.5	1124; 1.5	1088; 1.5	1125; 1.6	1050; 1.4
Wastewater Generation (m^3/day; gal/GGE fuel)[3,4]	917; 1.4	917; 1.4	948; 1.3	975; 1.3	1800; 2.5	932; 1.3

Table Notes:

1. The only difference between the 2009 and 2012 SOT cases is a decrease in hydrotreating catalyst consumption for the 2012 SOT.
2. Fossil energy consumption does not include grinding of the feedstock prior to the pyrolysis step.
3. Water consumption and wastewater generation include only direct use/emissions and do not include water associated with upstream production of materials and energy used at the plant.
4. Wastewater generation includes both wastewater from hydrotreating and blowdown from the cooling towers.

- Task 1.2.2 (TEA/LCA Framework)
- Task 2.2.2 (TEA/LCA Feedback)
- Task 3.2.3 (Full TEA/LCA Analysis)

Approach

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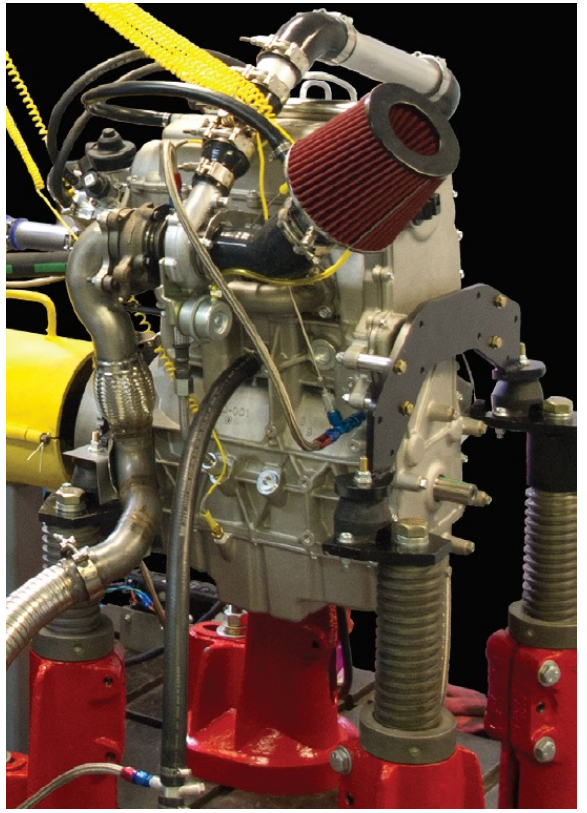
Engine Testing

- The technical approach to engine testing consists of dynamometer testing on a fully instrumented research engine.
- Mainstream Engineering will install its diesel research engine in the test cell and perform engine testing with fuels containing bio-based blendstocks produced by the project team.
- The engine, referred to as the AMD, is a bespoke three-cylinder, 1.25-L turbodiesel engine. It uses high-pressure common-rail fuel injection typical of modern automotive diesels. The open engine controller platform allows full authority control over the injection timing, rail pressure, and manifold air pressure.
- The AMD engine will be coupled to Mainstream's 120-hp AC-regenerative dynamometer.
- Baseline testing will be performed with neat diesel.
- The tests will then be repeated with the bio-based blends.
- Mainstream will measure exhaust gas temperatures, fuel-air ratio, gas emissions (CO, CO_2, NO/NOX, THC), particle emissions (PM mass and PM number), fuel consumption, brake torque, engine speed, and brake power (calculated). The brake fuel conversion efficiency (bsfc) and brake mean effective pressure (bmep) of the engine will also be calculated from measured quantities.



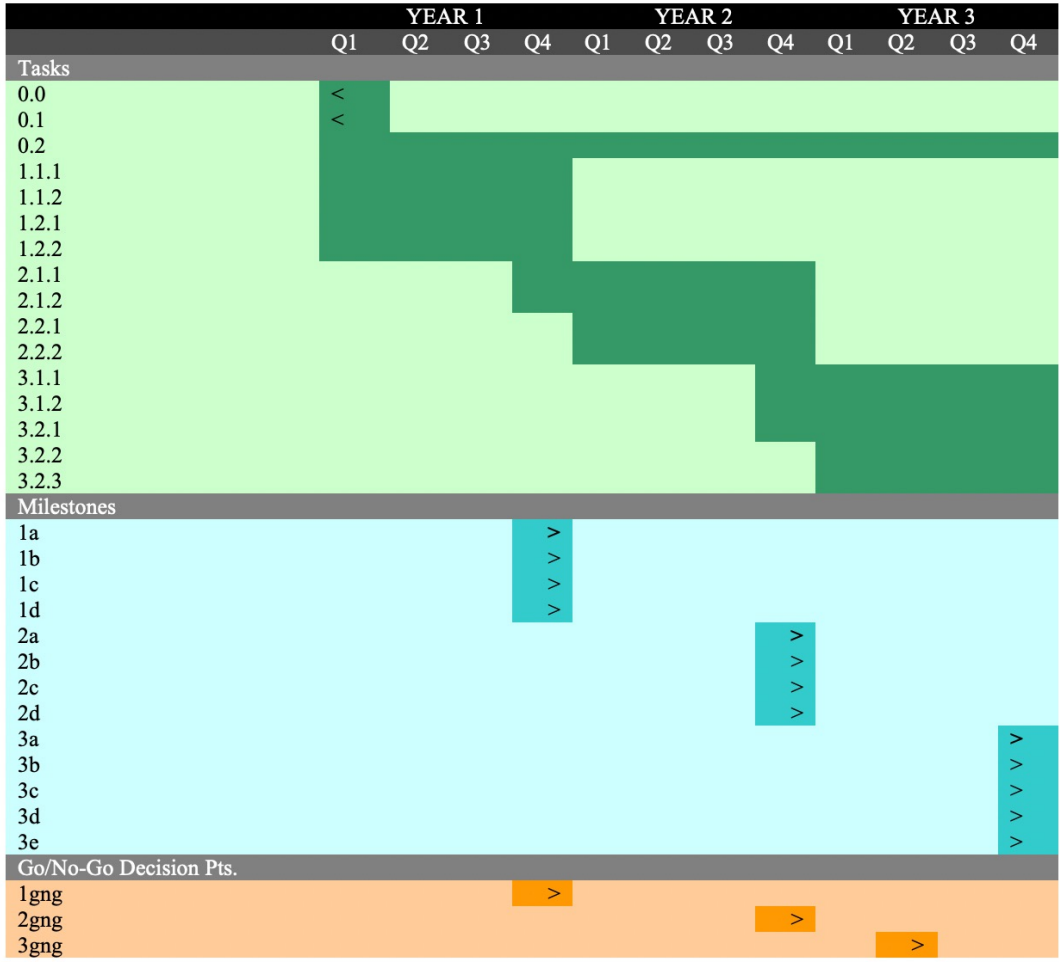
- Task 3.1.1 (Engine Testing)

Approach

Co-Optimization of Fuels & Engines

- **Challenges**
  - Laboratory access limited since March 2020 due to COVID-19 restrictions
  - Bio-oil throughput limited by delivery of bench-scale continuous reactor pyrolysis unit (production delayed)
  - The proposed catalytic upgrading relied on commercial tungstated zirconia catalysts, which were promised by a supplier but never delivered. Eventually we decided to synthesize and characterize our own materials.

- **Go/No-Go Decision Points**
  - 1gng: Demonstration Conversion/Upgrading Success
    - Phenol acylation demonstrated at greater than 90% phenol conversion and greater than 70% selectivity to acylated products
  - 2gng: Demonstration of Optimal Bioblendstock Properties
    - Identification of a bioblendstock that demonstrates a CN > 40 with a 10% reduction in sooting propensity
  - 3gng: TEA/LCA Validation
    - Estimated bioblendstock production capability at < $3.50/gge



Successfully completed 1gng, entered BP2 in 06/2020

Approach

Co-Optimization of Fuels & Engines

- **Economic and Technical Metrics**
  - Ability to blend into base diesel fuel at no less than 5% by volume
  - Achieve lifecycle greenhouse gas reductions of at least 50% compared to baseline
  - Use of suitable feedstock(s) as defined by the Energy Policy Act (EPACT) of 2005, Section 932(a)(1) and (2)
  - Improved energy density of >42 MJ/L, representing a 5-15% improvement over the baseline (typically 36-40 MJ/L)
  - Reduction in sooting propensity of >10%, as defined by Yield Sooting Index, over baseline (e.g. 111.4 for diesel fuel)
  - Improved cetane number of >40 as defined by Co-Optima targets
  - A bioblendstock that meets ASTM D975 Standard Specification for Diesel Fuel Oils
  - Production of a minimum of 500 ml of the identified bioblendstock to the national laboratory Co-Optima team to facilitate independent verification of fuel properties and performance. If possible, 10 gallons will be provided for more thorough evaluation.
  - A comprehensive techno-economic analysis (TEA) and a Life-Cycle Assessment (LCA) of the biofuel production pathway(s) for identified bioblendstock(s).
    - 3gng: Estimated bioblendstock production capability at < $3.50/gge
  - Single (or multi-cylinder) engine testing of the identified bioblendstock blended at >5% by volume with conventional petroleum-derived diesel, evaluated with respect to baseline performance of torque, fuel consumption, and relevant emissions.

Impact

Co-Optimization of Fuels & Engines

Successful completion of the project will provide:

- A bio-derived blendstock capable of operating efficiently in existing Diesel engines, thus reducing engine-out emissions
- A bio-derived blendstock that can be economically produced at scale using available biomass resources
- A bio-derived blendstock that can enable next-generation MCCI (Mixing-controlled Compression Ignition) and ACI (Advanced Compression Ignition) engines through properties superior to conventional Diesel

Dissemination of results through:

- Active participation in the multi-institution Co-Optima program
- Publication of results in high-impact journals
- Presentation of findings at national and international conferences
- Involvement with stakeholders in the transportation energy, including fuel companies, automobile companies, and distributors

Co-Optima Goal: Better Fuels and Better Vehicles Sooner

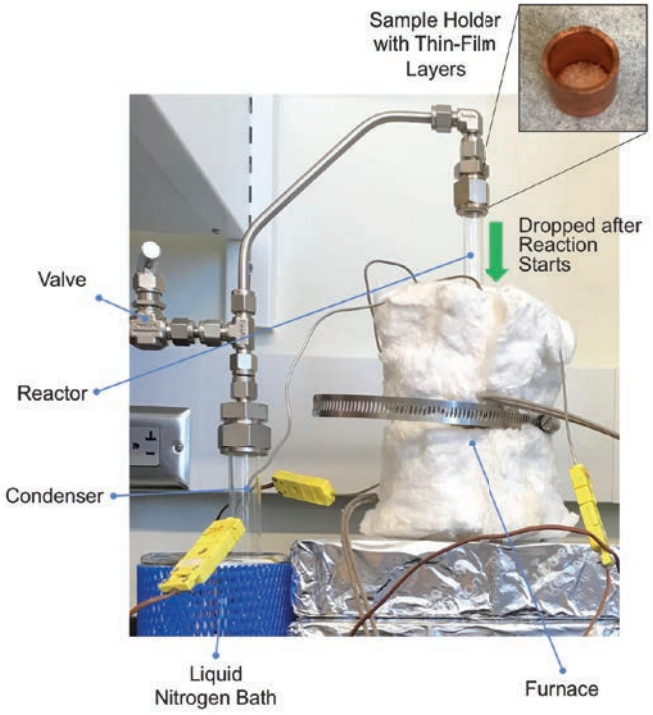
- *"What fuel properties maximize engine performance?"*
- *"How do engine parameters affect efficiency?"*
- *"What fuel and engine combinationsare* ***sustainable, affordable, and scalable****?"*

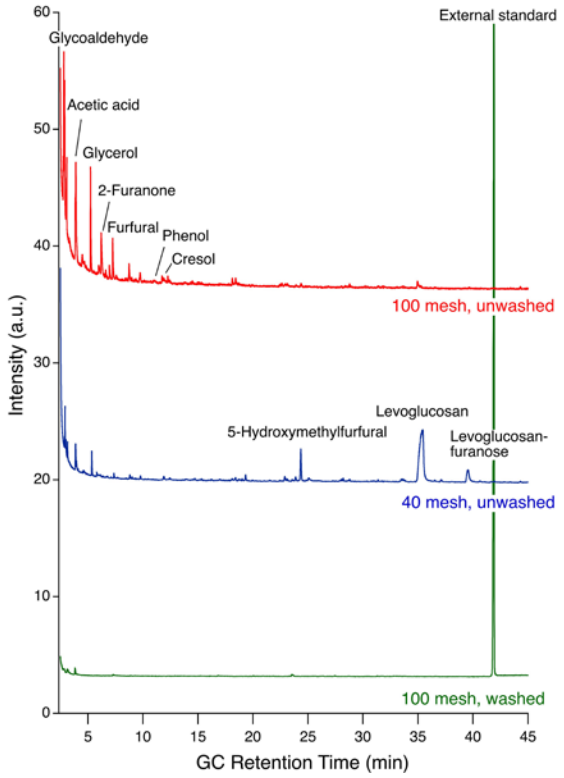
Progress & Outcomes

Co-Optimization of Fuels & Engines

Identify optimal mixing patterns and biomass feedstocks for fast pyrolysis

- Based on our experiments, the size of the actual sawdust samples was identified as a major factor to affect the product distributions of the resultant bio-oils.
- Particularly, sawdust with a particle size of as small as 100 mesh (i.e., smaller than 150 micron), without the removal of its native mineral, produces bio-oils containing suitable molecules for subsequent upgrading (acetic acid, furfural, phenol, and cresol, estimated to be approximately 20-30 wt% in total).
- Particle size in the ideal range identified by NREL for pyrolysis (< 2-3 mm)





Milestone 1a: Identify the optimal mixing patterns and feedstock types of sawmill residues for producing the pyrolysis-derived bio-oil that is most upgradable, or if used directly, has the best combustion properties.

Progress & Outcomes

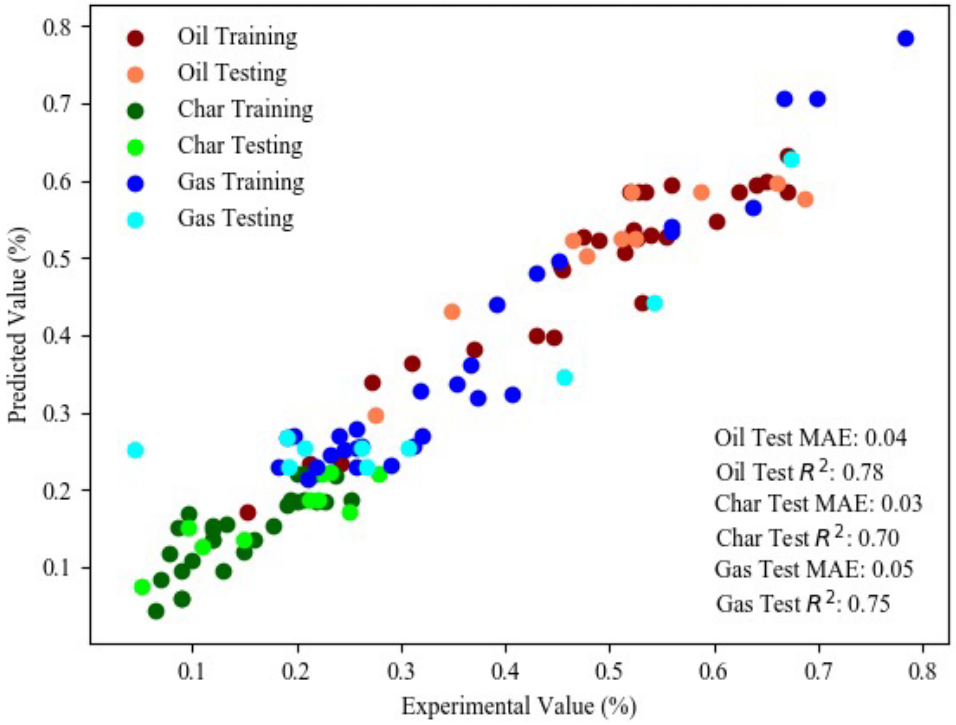
Co-Optimization of Fuels & Engines

Parametric expression of bio-oil compositions on feedstock properties and reactor operation conditions

Milestone 2a: Parametric model is able to predict within 10% of the product yields from the fast pyrolysis experiments

Bio-oil yields

- More than 50 papers have been reviewed, and the data within the papers were compiled into a database
- The database tabulates *feedstock properties* and *reactor operation conditions* as inputs and *yields of gases, bio-oil, char*, as well as of *individual products* as outputs for subsequent development of parametric expressions
- The Artificial Neural Network (ANN) methodology developed by the Mack group was used to map the inputs and outputs for the parametric expression



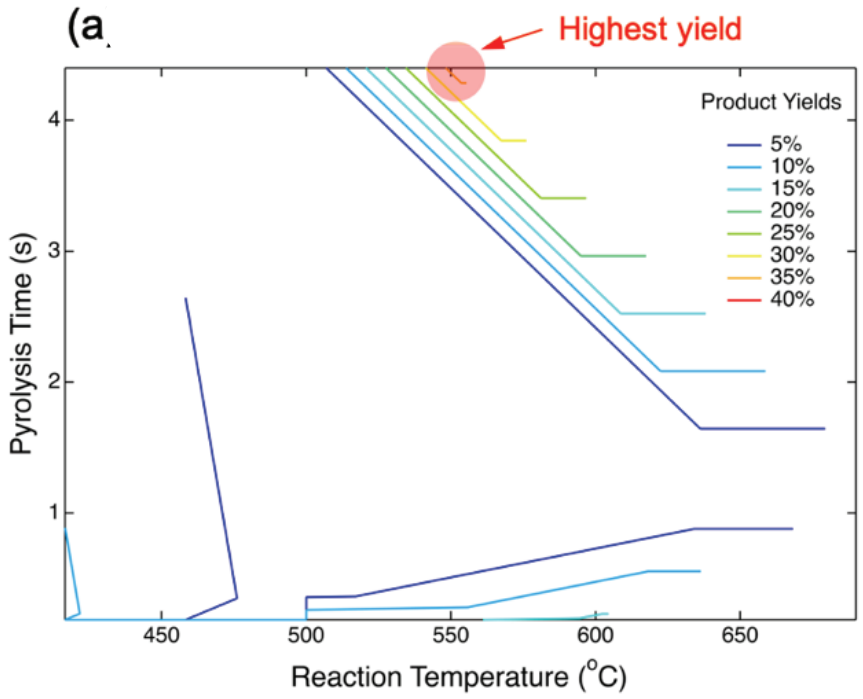
*The ANN achieves a test set prediction r-squared correlation coefficient of 78%, 70%, and 75%, and a test set median absolute error of less than **4%**, **3%**, and **5%**, for bio-oil, char, and gaseous yields, respectively.*

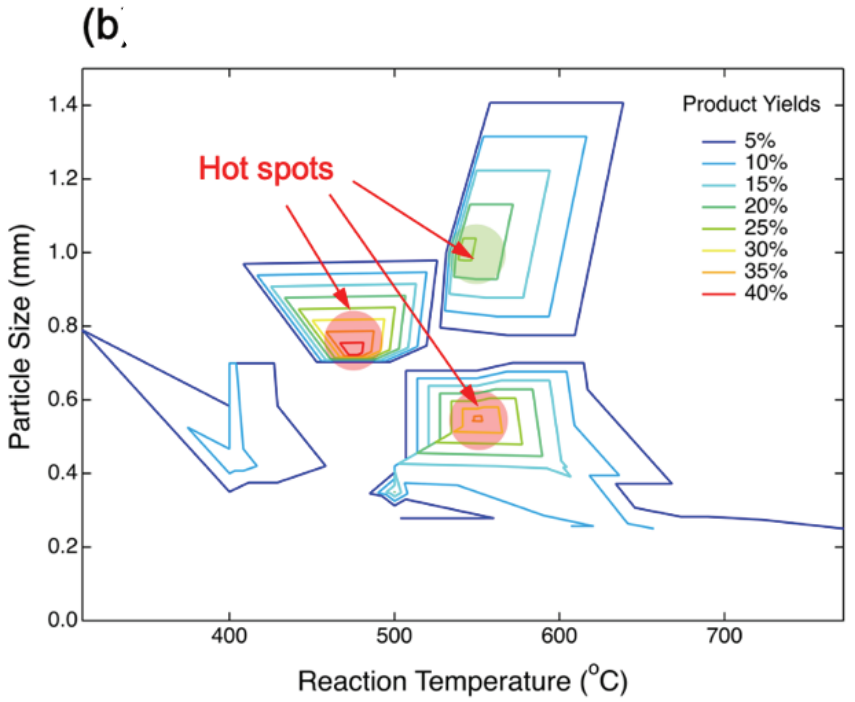
Progress & Outcomes

Co-Optimization of Fuels & Engines

Parametric expression of bio-oil compositions on feedstock properties and reactor operation conditions

Milestone 2a: Parametric model is able to predict within 10% of the product yields from the fast pyrolysis experiments





Parametric dependence of the yields of aromatic alcohols (on reaction time, temperature, and particle size)]

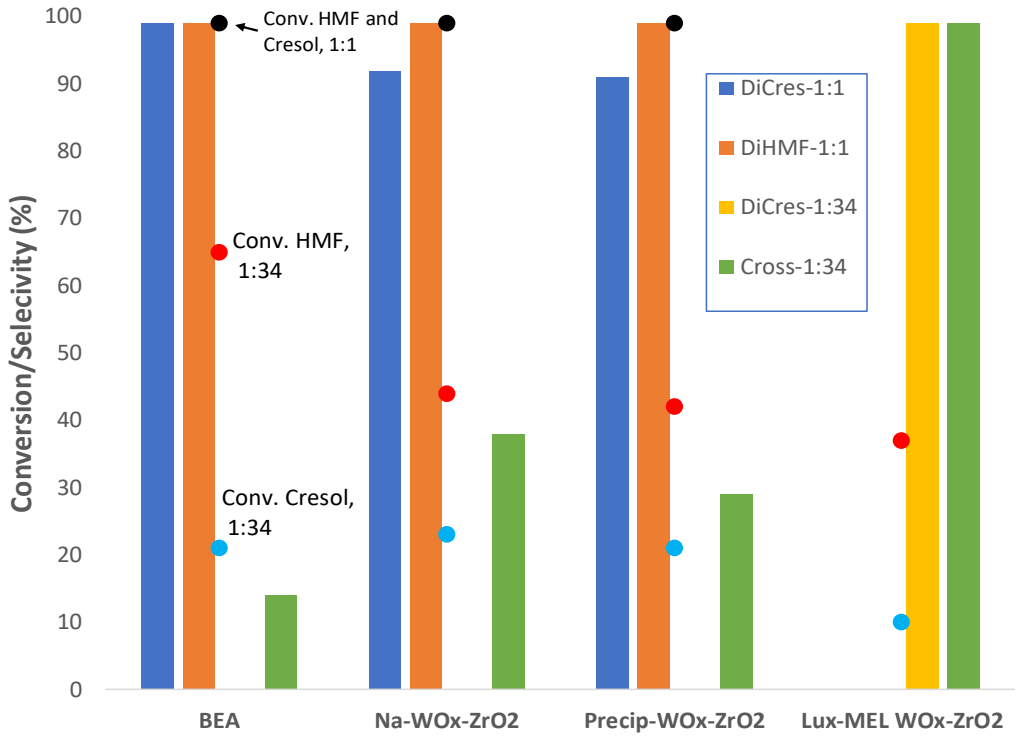
Analysis focused on fluidized bed reactors due to their commercialization promise (continuous operation). Other reactors also considered in future work.

Yields of individual products are more challenging to model through ANN with all inputs considered, due to lack of data (sparser matrices). Selected parameters (reaction temperature, time, and biomass particle size) were used to determine the correlations

Progress & Outcomes

Co-Optimization of Fuels & Engines

Catalytic Upgrading – Etherification of furans with phenolics



- Conversion and selectivity obtained with various catalysts:
  - BEA Zeolite
  - Two in-house WO_x-ZrO_2 catalysts.
  - Commercial WO_x-ZrO_2 from Luxfer-MEL
- Reactions were run with either excess *o*-cresol or 1:1 HMF and cresol.
- Excess *o*-cresol causes catalyst deactivation and low selectivity.
- Can achieve high selectivity by using 1:1 HMF:cresol.
- Better solution: hydrogenate bio-oil before doing etherification to *prevent* deactivation.

Milestone 1b: Cresol etherification demonstrated at >90% cresol conversion and >70% selectivity to etherified products using model compounds.

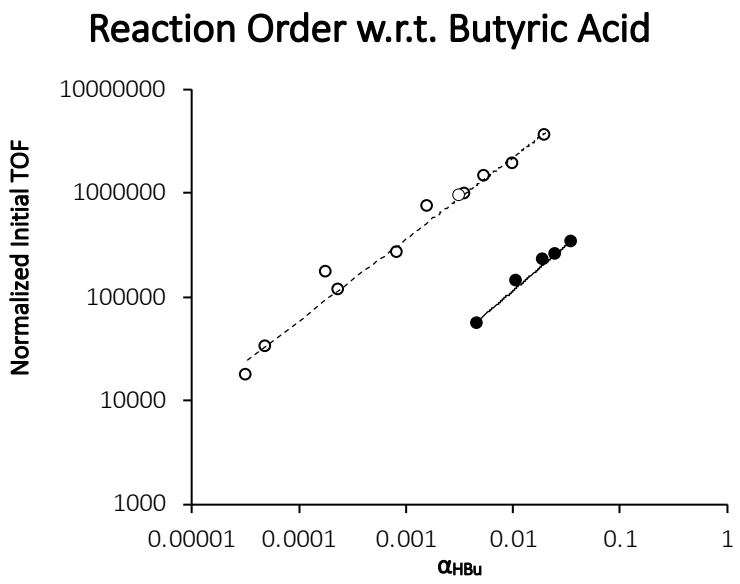
Demonstrated >95% conversion and > 95% selectivity.

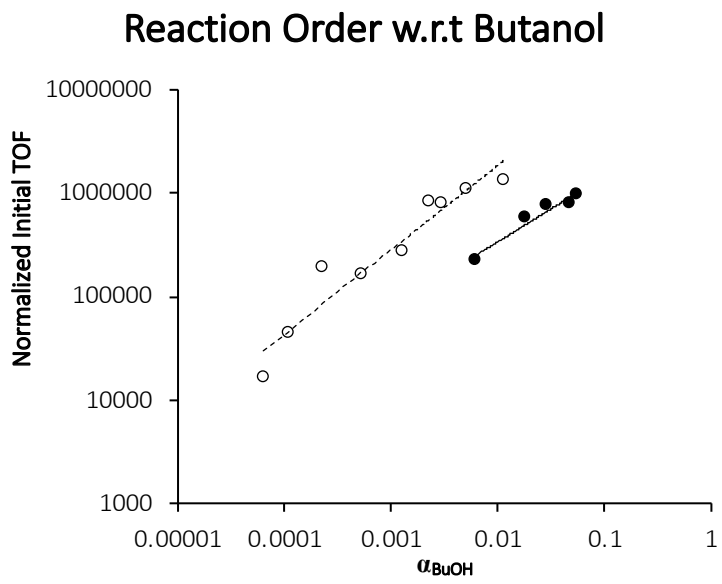
Progress & Outcomes

Co-Optimization of Fuels & Engines

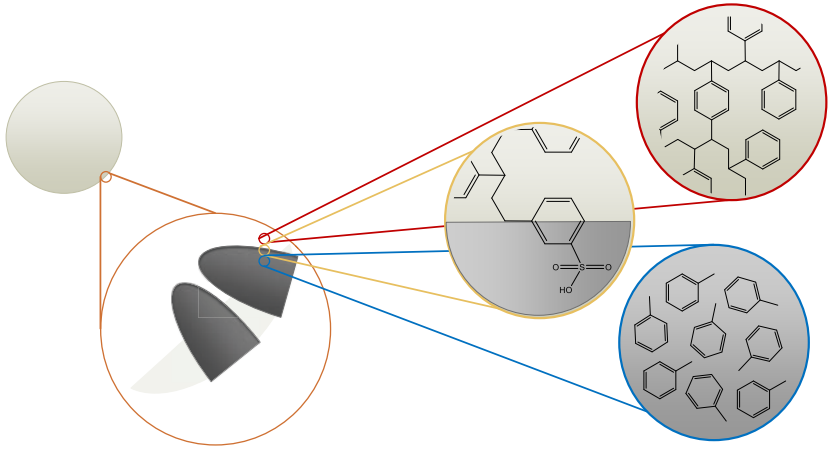
Catalytic Upgrading – Analysis of Esterification Data

We analyzed previously-collected data for **catalytic esterification**, which will be an **important side reaction** when working with *real bio-oil* that has both acids and alcohols.





Two different acid catalysts, Amberlyst 46 (○) and Amberlyst 15 (●), were evaluated. Reaction orders are the same over both catalysts, but the turnover frequency (TOF) decreases when using A15. These should be identical!

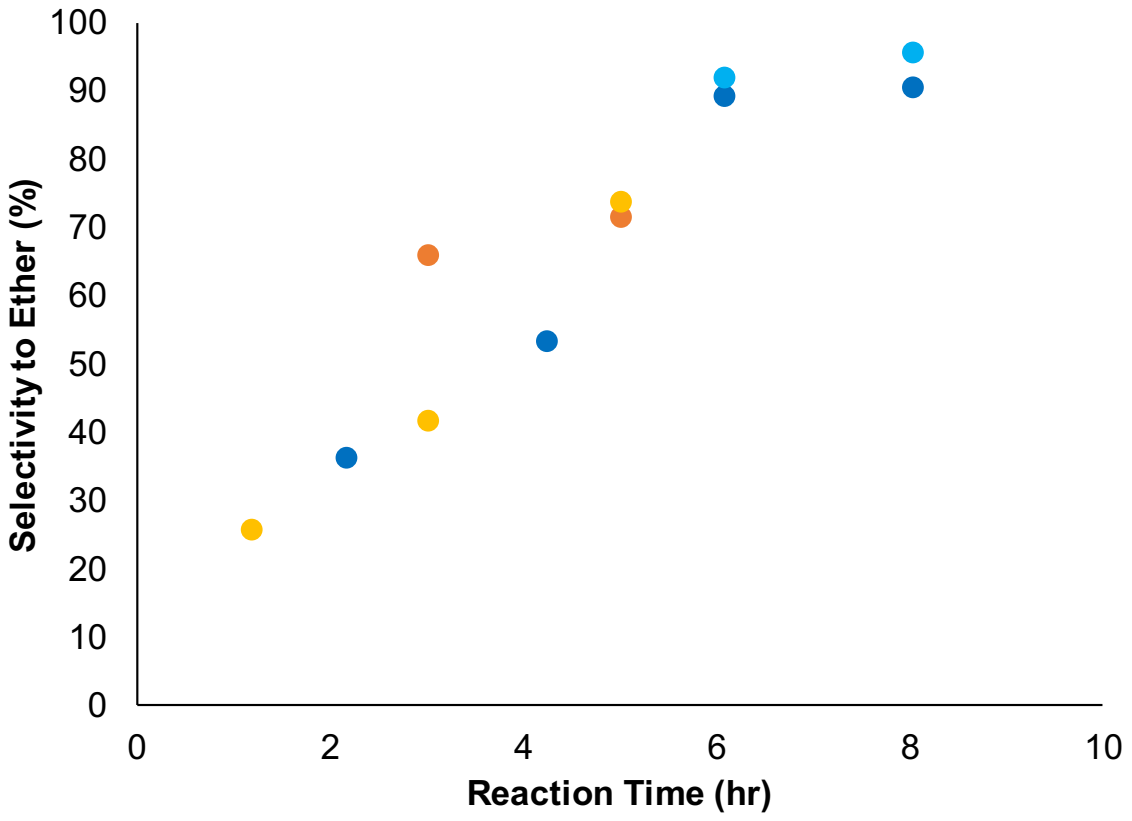


The discrepancy in rates appears to be caused by solvation of reactive species by the catalyst itself! Ongoing work seeks to verify this hypothesis. *This could allow us to tune reactivity, possibly also for etherification.*

Progress & Outcomes

Co-Optimization of Fuels & Engines

Catalytic Upgrading – Etherification of Hydrogenated Species



Achieved **high selectivity to ether products**, which shows that production of ethers for fuel blending can be accomplished by reacting previously-hydrogenated molecules.

Ongoing work:

- Hydrogenation of aromatics + furans – This is being evaluated using Pd/C. Preliminary results suggest high selectivity, but further analysis is needed.
- Etherification of hydrogenated species – Evaluating potential for intermediate products (suggested by increase in selectivity w.r.t. reaction time)

Milestone 2b: Hydrogenation of ether derivatives demonstrated at greater than 90% conversion of ether and greater than 70% selectivity to saturated products using feedstocks produced according to Task 1.1.2, originally derived from real bio-oil

Progress & Outcomes

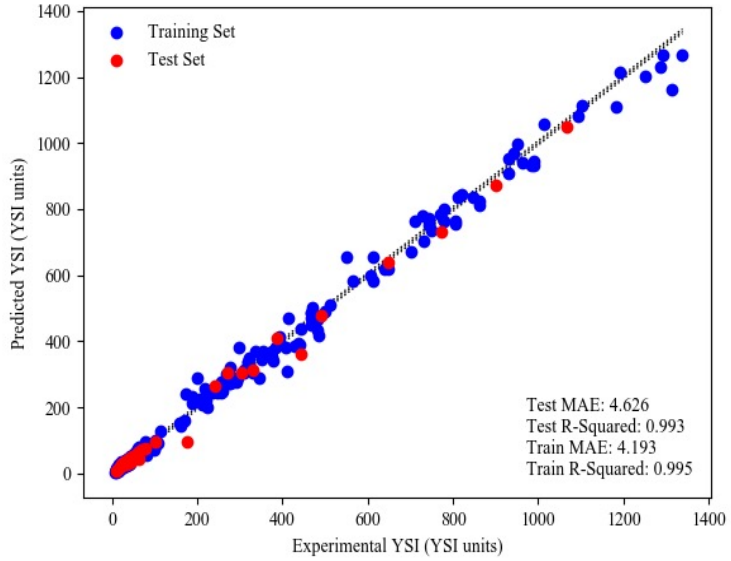
Co-Optimization of Fuels & Engines

Property Evaluation & Feedback

- Developed custom models for CN, RON, MON, YSI, energy density, cloud point, and kinematic viscosity
- Advancements include **improved accuracy** and a **comprehensive** set of models for fuel properties
- Created comprehensive databases of experimental values for each property from literature sources (including the Co-Optima Property Database), which were used in model development
- Artificial Neural Network (ANN) accuracy, defined by the median absolute error (MAE) of test set predictions, for each of the properties is shown in the table below
- Median absolute error for test set predictions are well below 4% error.

Milestone 1c: Model performance for CN, YSI, and other indicated properties of interest at a median absolute error (MAE) of < 4%.

Property Name	Range (Experimental Max. – Min.)	Test Set MAE	% Error
Cetane Number	167 CN units	4.048	2.42%
Research Octane Number	120 ON units	3.673	3.06%
Motor Octane Number	112.3 ON units	2.952	2.62%
Yield Sooting Index	1332.3 YSI units	4.626	0.35%
Kinematic Viscosity	6.63 m^2/s	0.045	0.68%
Cloud Point	94.3 °C	0.605	0.64%



Progress & Outcomes

Co-Optimization of Fuels & Engines

Property Evaluation & Feedback

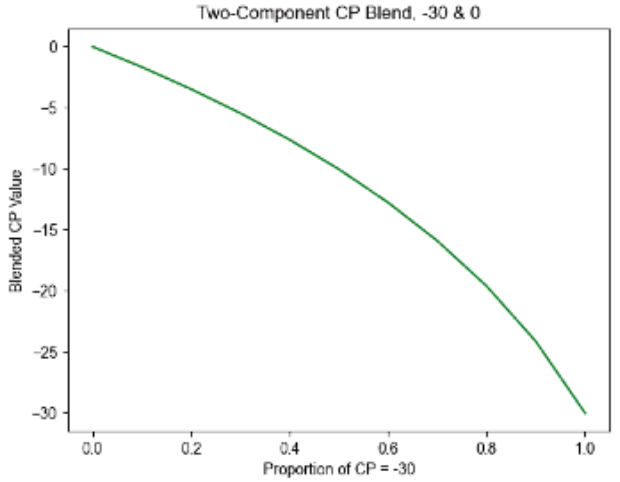
- Approach to Multi-Component Blend Predictions
  - Predict individual component properties
  - Calculate blend value using linear & non-linear equations
  - Individual prediction errors propagated through equations, obtain expected blend error

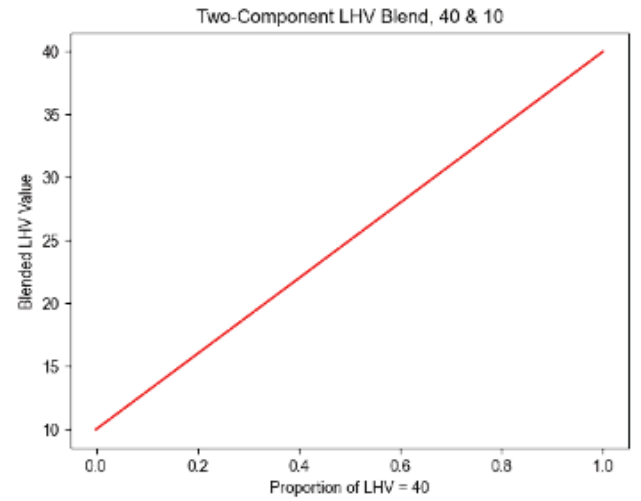
- The approach successfully predicts blend properties of other bioblendstocks

Blend	CN	Pred. CN	YSI	Pred. YSI	LHV (kJ/l)	Pred. LHV	KV (cSt)	Pred. KV
Soy Biodiesel	52	50.3870	80	96.0678	33	25.5023	4.054	4.7067
POME	73	63.0231	2.1	16.3542	19.3	11.5965	1.19	1.2239

- Average prediction error < 5%
  - Calculated using absolute error, known experimental property value ranges

Milestone 2c: Modeled properties for actual bioblendstocks at <5% error; feedback for conversion and upgrading processes





Progress & Outcomes

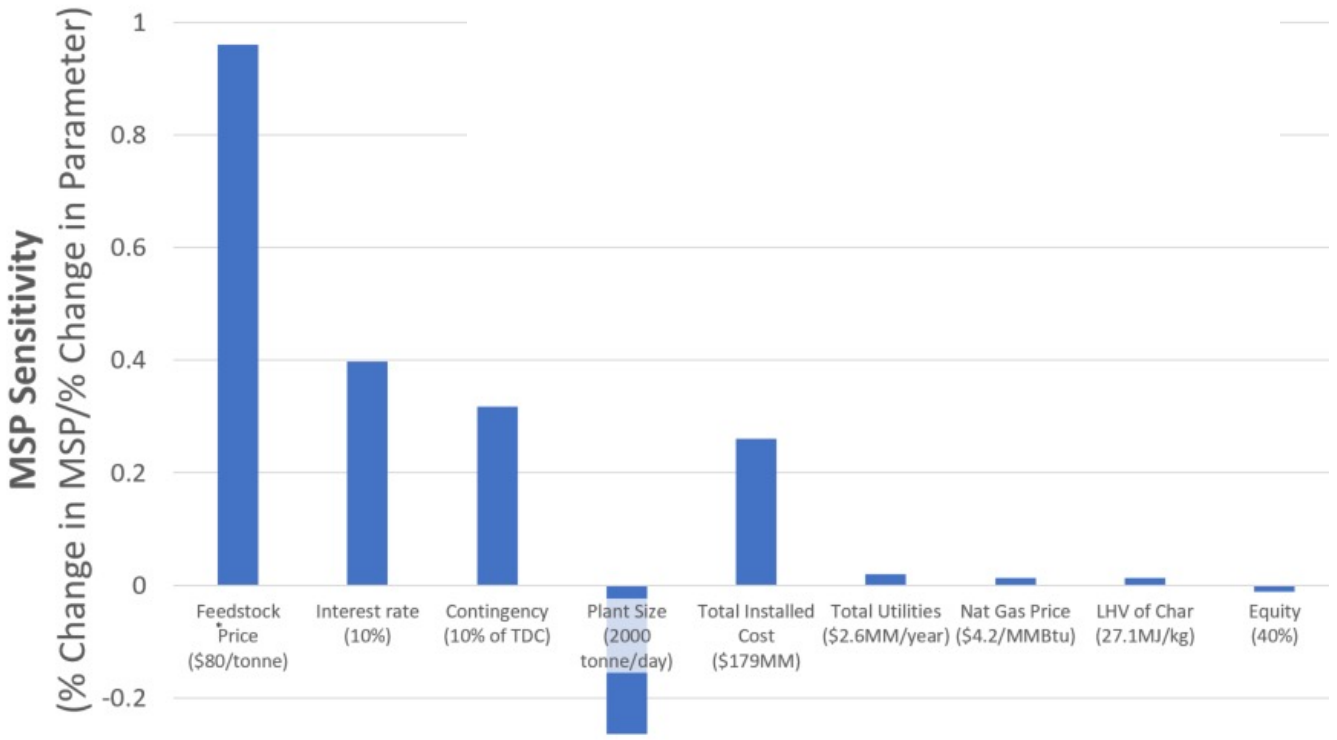
Co-Optimization of Fuels & Engines

Techno-economic Analysis

Milestone 1d: TEA/LCA Framework

The process was simulated in Aspen using predicted yields for each process step, and the capital and operating costs were used to estimate the Minimum Selling Price for a Diesel Gallon Equivalent (DGE) blendstock.

- **Economic assumptions** and calculations consistent with Dutta (2015)
- **Etherification model compounds'** thermodynamic properties determined using Density Functional Theory
- **Overall yield** = 84 DGE/tonne (55 million DGE/y)
- **Minimum selling price (MSP)** = $2.37 per DGE
- **Capital cost** = $6.5 per annual DGE



*values in parentheses were used to calculate the base case MSP

Milestone 2d: TEA/LCA Feedback (in progress)

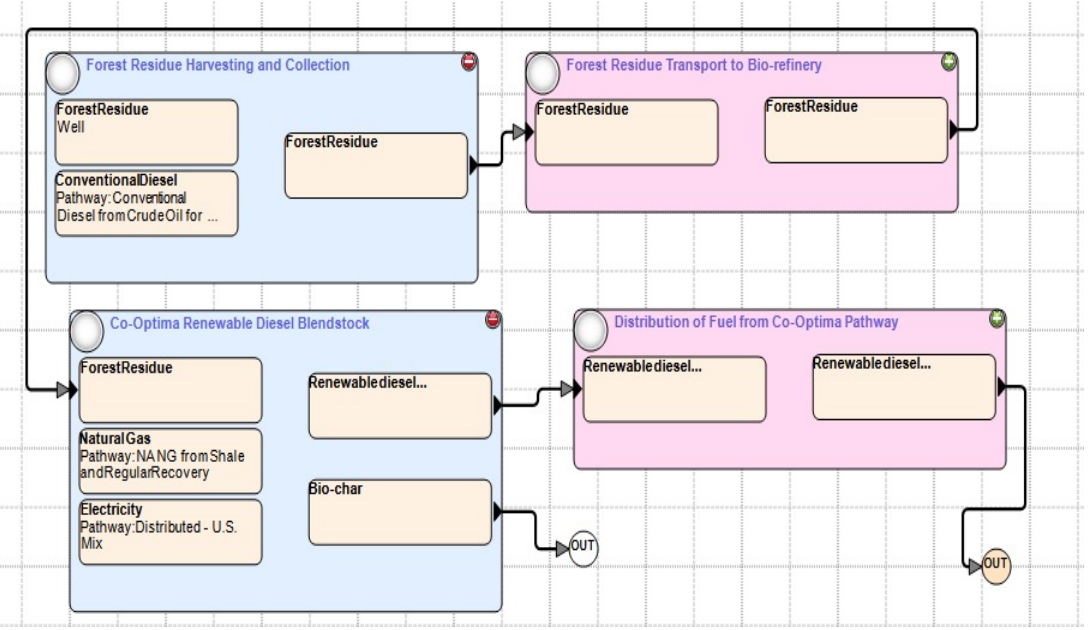
- TEA/LCA Models being revised to account for mild hydrogenation of the pyrolysis oil prior to etherification.
- Sensitivities to feedstock variations and process yields are being conducted.

Progress & Outcomes

Co-Optimization of Fuels & Engines

Life-Cycle Assessment

Co-Optima pathway simulated in GREET 2019.net



- ✓ **2,000 tonne** of forest residues consumed **5,280 gallons** of conventional diesel
- ✓ **494 million Btu** of natural gas was used to provide the steam used in the Aspen simulation
- ✓ The products include **23 TJ** of renewable diesel blendstock and **2.42 TJ** of bio-char
- ✓ Renewable diesel blendstock was transported 200 miles to the pump consuming **1,460** gallons of conventional diesel

Well to Wheels Comparison of Co-Optima Renewable Diesel Blendstock to Conventional Diesel for Base Case

		Conventional Diesel	Co-Optima Blendstock	% Reduction
Energy Use	**Units**			
Total Fossil Fuel	MJ/DGE	164.4	13.1	92%
Coal	MJ/DGE	2.1	0.1	
Natural Gas	MJ/DGE	18.6	4.1	
Petroleum	MJ/DGE	143.8	8.9	
Emissions				
Volatile Organic Compounds	g/DGE	6.3	5.9	6%
Carbon Monoxide	g/DGE	19.0	18.7	2%
Nitrogen Oxides	g/DGE	131	131	0%
Particulate Matter 10mm	g/DGE	4.0	3.9	2%
Particulate Matter 2.5mm	g/DGE	3.8	3.8	2%
Sulfur Oxides	g/DGE	3.4	2.8	18%
Methane	g/DGE	23	23	2%
Nitrous Oxide	g/DGE	0.3	0.3	2%
Carbon Dioxide	g/DGE	11828	44*	100%
Greenhouse Gases (CO2e)	g/DGE	12639	836*	93%

*After credit for biogenic CO_2 emissions from end use

As the results illustrate, the renewable diesel blendstock has a 92% reduction in total fossil fuel energy use and a 93% reduction in greenhouse gas emissions relative to petroleum diesel.

Summary

Co-Optimization of Fuels & Engines

1. **Overview:** The project team proposes an integrated approach to the development and production of bioblendstocks that improve the energy density, sooting propensity, and cetane number of base diesel fuel while maintaining cold weather behavior
2. **Approach:** The process converts sawmill residues into bio-oil through selective fast pyrolysis; the bio-oil is then selectively upgraded to form selectively oxygenated, minimally-branched hydrocarbons using non-noble metal catalysts in combination with metal-catalyzed hydrogenation. Advanced predictive models, in conjunction with existing property databases, and experimental testing are used to evaluate overall bioblendstock properties and their impact on base diesel fuel.
3. **Technical Accomplishments / Progress / Results:** Successfully demonstrated the conversion of woody biomass to bio-oil and understood the driving parameters influencing yield/composition. Showed high conversion and selectivity during upgrading process to desired molecules. Developed accurate pure component and blend models for fuel properties. Integrated process into TEA/LCA frameworks for evaluation and process feedback.
   - On track to realize the target economic and technical metrics (Slide 10)
   - Energy density of >42 MJ/L is aggressive; >25 MJ/L meets the Co-Optima criteria
4. **Relevance:** The economic production of a bio-derived blendstock will reduce engine-out emissions, life-cycle impacts, and increase engine efficiency.
5. **Future Work:** Scale-up of bio-oil production and catalytic conversion of resultant bio-oils, experimental evaluation of actual bioblendstock, and engine testing.

Quad Chart Overview

Timeline

- Project start date: 10/1/18
- Project end date: 5/31/22

	FY20 Costed	Total Award
DOE Funding		$1,001,932
		$451,785

Project Partners

- University of Massachusetts Lowell
- University of Maine
- Mainstream Engineering

Project Goal

The goal of this project is to economically and sustainable produce bioblendstocks that improve the energy density, sooting propensity, and cetane number of base diesel fuel while maintaining cold weather behavior.

End of Project Milestone

- **End of Project Goal #1:** Develop a multicomponent liquid bioblendstock for use in medium- and heavy-duty mixing controlled, compression ignition engines blended into a base diesel fuel at no less than 5% by volume
- **End of Project Goal #2:** Provide a blendstock that reduces sooting propensity by 10% while providing a CN > 40
- **End of Project Goal #3:** Demonstrate operation of bioblendstock in an engine without degradation in performance or emissions relative to conventional diesel fuel

Funding Mechanism

- Fiscal Year 2018 Advanced Vehicle Technologies Research Funding Opportunity Announcement (DE-FOA-0001919)
- AOI 5b: Bioblendstocks to Optimize Mixing Controlled Compression Ignition (MCCI) Engines

Additional Slides

Responses to Previous Reviewers' Comments

Co-Optimization of Fuels & Engines

- 2019 DOE BETO Peer Review
  - Presented an overview poster since the project was newly funded
  - "Technically this project is good with right combination of experts running the project. One of the strong points of this project is, the team is considering production and testing a mixture of chemical compounds, which is good from economic and mass production point of view. This project clearly aligns with BETO goals and objectives. The successful completion of this project would definitely help fuel industry to introduce the outcomes in commercial diesel production with bio component." (Reviewer #1)
  - "In order to reduce the cost of producing biofuels from pine biomass, this project will test the performance of partially oxygenated hydrocarbons as biofuels to reduce production costs, which seems to be an interesting idea. An iterative upgrading approach coupled with technoeconomic assessments, life cycle analyses, and machine learning prediction software will be deployed to determine the optimal conditions to obtain cost-effective biofuel products." (Reviewer #2)

- Go/No-Go Decision Point #1
  - Successfully cleared GNG1 in May 2020
  - Entered into Budget Period 2 in June 2020

Publications, Patents, Presentations, Awards, and Commercialization

Co-Optimization of Fuels & Engines

Publications

- Kessler, Travis, Peter C. St John, Junqing Zhu, Charles S. McEnally, Lisa D. Pfefferle, and J. Hunter Mack. "A comparison of computational models for predicting yield sooting index." *Proceedings of the Combustion Institute* (2020).
- Sharma, Sanskriti, Hernan Gelaf-Romer, Travis Kessler, and John Hunter Mack. "ECabc: A feature tuning program focused on Artificial Neural Network hyperparameters." Journal of Open Source Software 4, no. 39 (2019): 1420.
- Huo, Xiangchen, Nabila A. Huq, Jim Stunkel, Nicholas S. Cleveland, Anne K. Starace, Amy E. Settle, Allyson M. York, J. Hunter Mack et al. "Tailoring diesel bioblendstock from integrated catalytic upgrading of carboxylic acids: a “fuel property first” approach." Green Chemistry 21, no. 21 (2019): 5813-5827.

Conference Proceedings

- Kessler, Travis, Thomas Schwartz, Hsi-Wu Wong, and J. Hunter Mack. "Predicting the Cetane Number, Yield Sooting Index, Kinematic Viscosity, and Cloud Point for Catalytically Upgraded Pyrolysis Oil Using Artificial Neural Networks." In ASME 2020 Internal Combustion Engine Division Fall Technical Conference. American Society of Mechanical Engineers Digital Collection, 2020.
- Kessler, Travis, Thomas Schwartz, Hsi-Wu Wong, and J. Hunter Mack. "Screening Compounds for Fast Pyrolysis and Catalytic Biofuel Upgrading Using Artificial Neural Networks." In Internal Combustion Engine Division Fall Technical Conference, vol. 59346, p. V001T02A007. American Society of Mechanical Engineers, 2019. [awarded Best Presentation Award]

Process Flow Diagram

Co-Optimization of Fuels & Engines