DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Polyoxymethylene Ethers (POMEs) as a High Cetane, Low Sooting Biofuel Blendstock for Use in MCCI Engines

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Bret Windom
Colorado State University

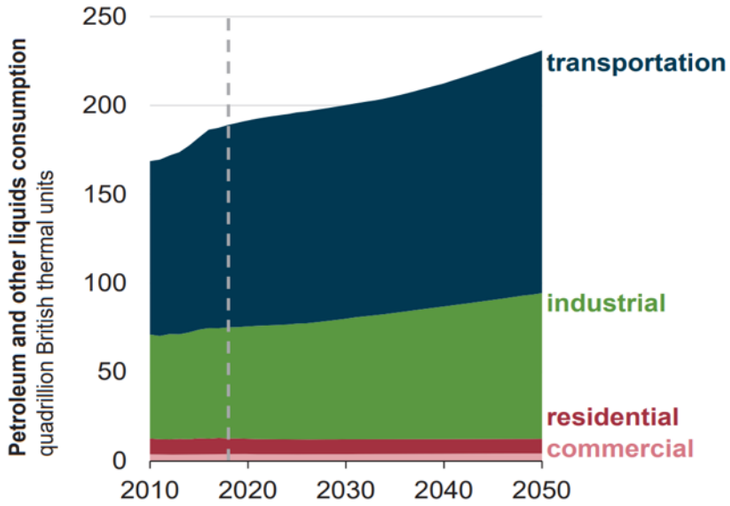
WALTER SCOTT, JR. COLLEGE OF ENGINEERING
COLORADO STATE UNIVERSITY

NREL Transforming ENERGY

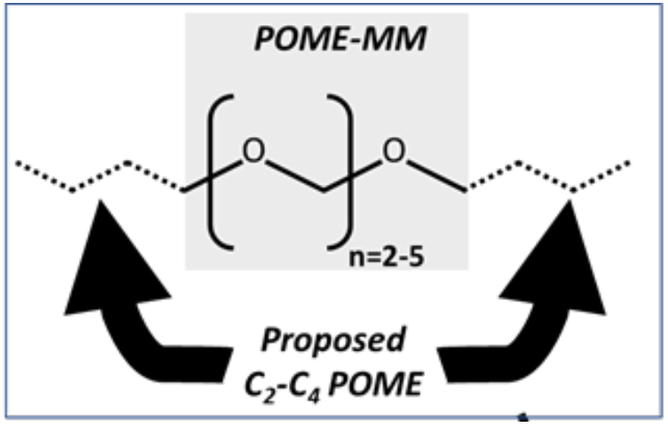
Project Overview

Background and Motivation

- Petroleum fuel consumption will continue to grow
  - Growth in non-OECD transportation sector will dominate
  - Significant growth in heavy-duty freight expected
- Modern Mixing Controlled Compression Ignition (MCCI) diesel engines used in heavy duty freight exhibit high thermal efficiencies but are plagued by **high NOx and particulate matter (PM) emissions**, and require costly and energy intensive exhaust aftertreatment systems
- Estimated 10.2 million premature deaths annually from fossil-fuel component of $PM_{2.5}$[1]
- **Renewable tailormade biofuels** have the ability to:
  - Reduce life cycle carbon emissions
  - Target fuel properties to enhance engine performance/efficiency and reduce emissions
  - Sourced from regional biomass
- ***Poly(oxymethylene) ethers (POME) with extended alkyl end groups***, exhibit favorable properties for use as a diesel fuel blendstock including:
  - ***Enhanced cetane numbers (CN)***
  - ***Significant soot reduction potential***
  - ***Acceptable lower heating values (LHV), oxidative stability, and water solubility***



From International Energy Outlook 2019

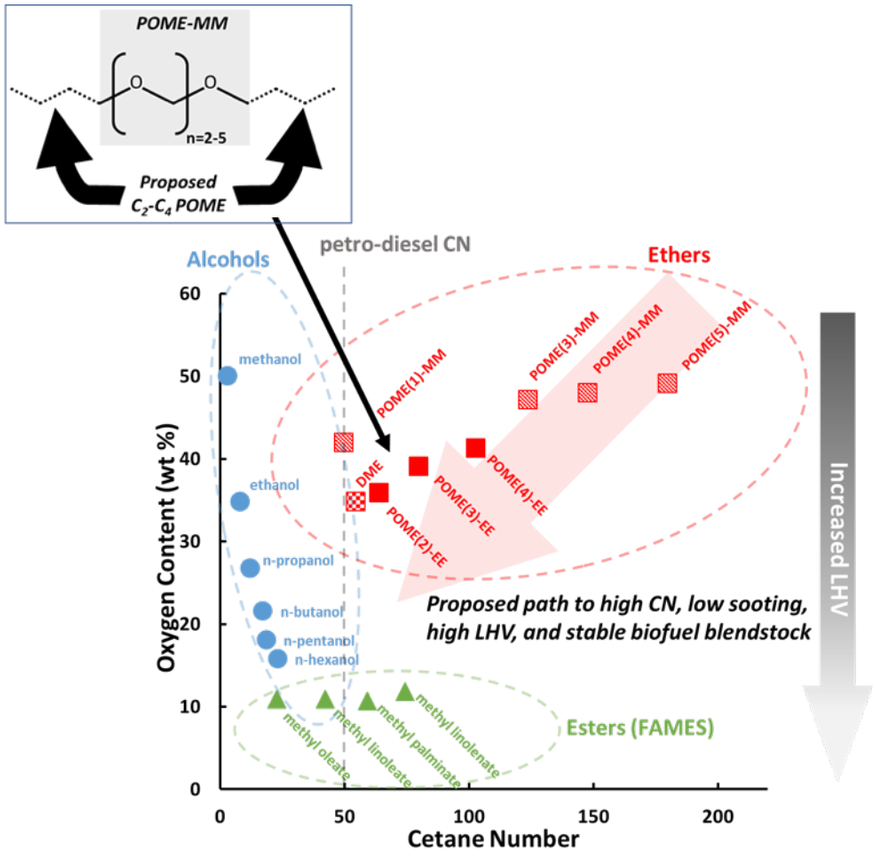


[1] Vohra, Karn, et al. "Global mortality from outdoor fine particle pollution generated by fossil fuel combustion: Results from GEOS-Chem." Environmental Research (2021): 110754.

Project Overview

Goals

- To synthesize a novel group of ***poly(oxymethylene) ethers (POMEs)*** with extended alkyl end functional groups capable of:
  - >50% reduction in life cycle GHG relative to conventional diesel
  - Significantly reducing soot emissions (i.e., reduce YSI)
  - Maximize energy density (i.e., maximize LHV)
  - Maintain compliance with ASTM D975 diesel fuel specifications.
- To identify the soot reduction potential, cetane number enhancement, and physico-chemical properties of POMEs.
- To identify an optimal biofuel blendstock comprised of the novel group of POMEs which present viable production pathways from lignocellulosic feedstocks
- To determine the ultimate potential of a POME MCCI fuel blendstock via TEA & LCA analysis, engine testing and consultation with industrial partner
- To investigate the scale-up of POME production and optimal usage (*i.e.*, combustion regime and appropriate emission reduction systems) in MCCI engines.

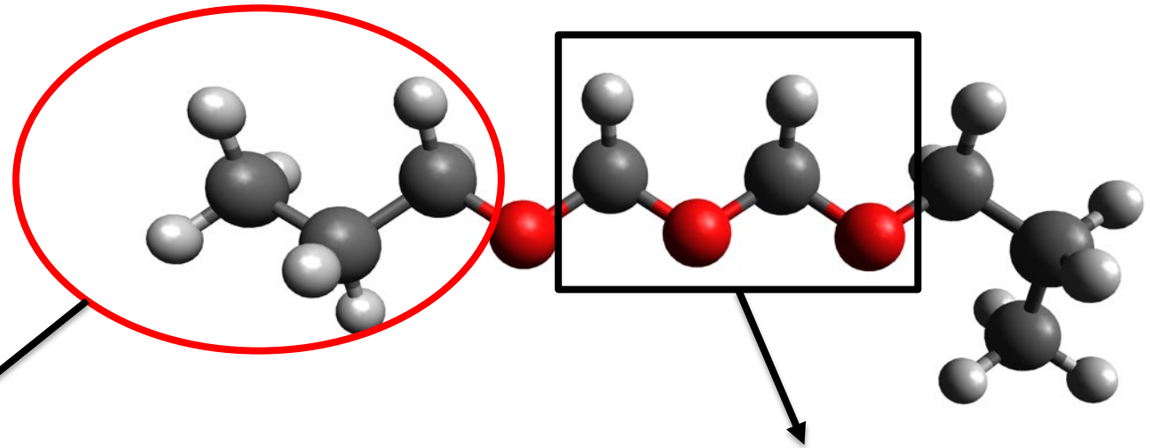


Tier Criteria	Greatly Exceeds	Exceeds Criteria	Meets Criteria	Barriers Exist
Cetane	> 50	46 to 50	40 to 45	< 40
LHV (MJ/kg)	> 40	31 to 40	25 to 30	< 25
Flash Pt (°C)	> 70	61 to 70	52 to 60	< 52
Melting Pt (°C)	< -50	-50 to -26	-25 to 0	> 0
Water Sol (mg/L)	< 5	5 to 501	500 to 1000	> 1000
YSI	< 50	50 to 151	150 to 200	> 200

MCCI merit table for blendstock screening

Overview - Nomenclature

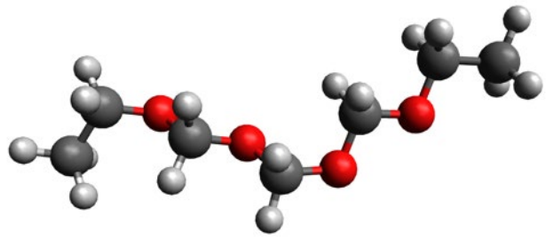
IUPAC Name: Propoxy(methoxy(methoxy))-propane (P-2-P)



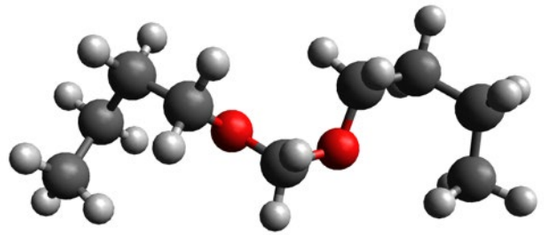
Alkyl end-groups are denoted as M, E, P and B for methyl, ethyl, propyl and butyl groups, respectively.

Numerical number represents the number of oxymethylene unit available in the backbone.

Other examples:



E-3-E



B-1-B

- Isomer and mixed end groups possible (e.g. B-n-M, iB-n-M, etc.)

1- Management

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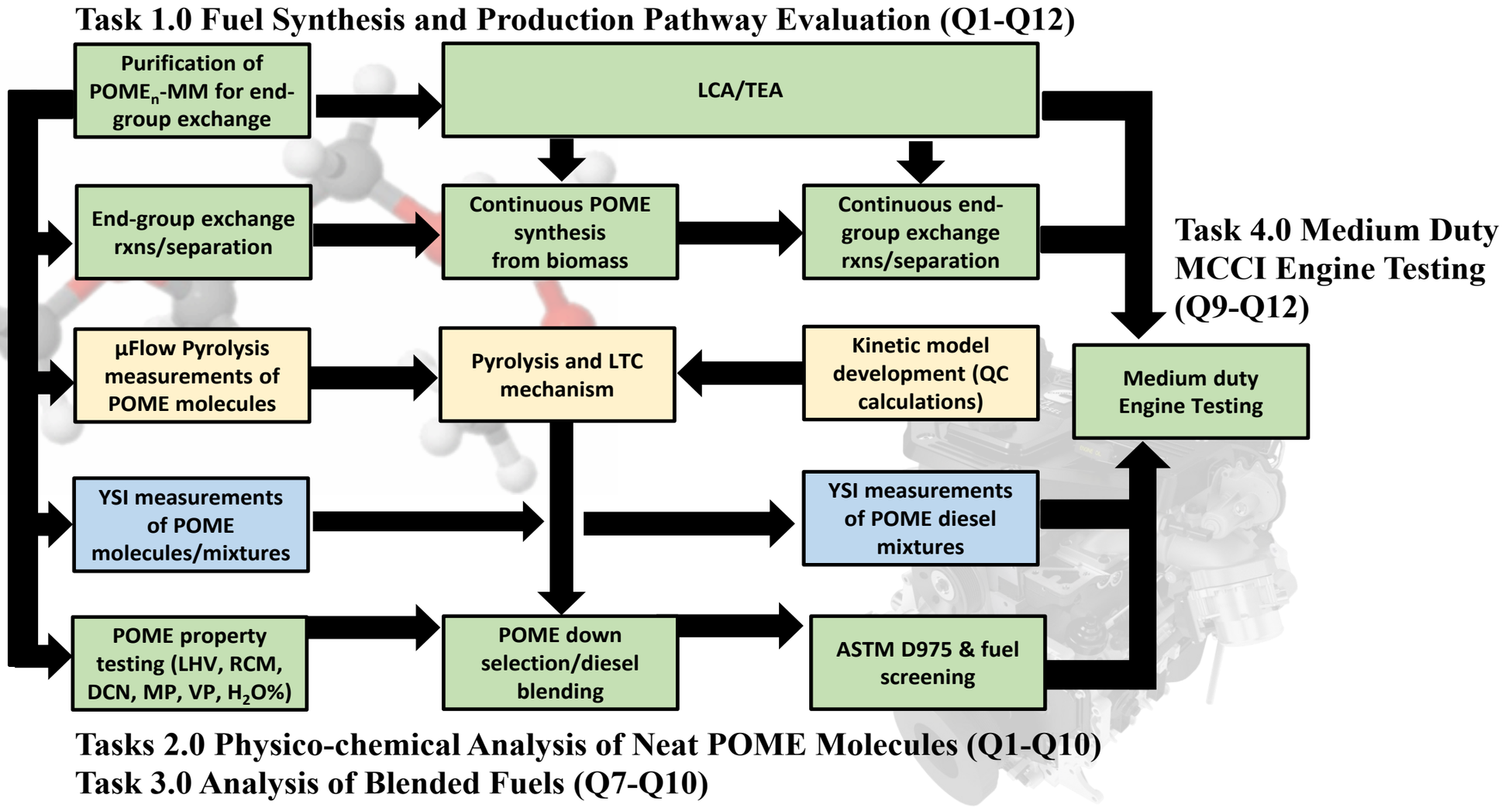
Yale



1- Management

Project Risks and Mitigation Strategies

- **Risk 1:** Compound synthesis, separation, and purification

  Implications: Prevent delivery of samples to project partners and halt project

  Mitigation: Partnering with NREL to use spinning band distillation and Simulated Moving Bed (SMB) Chromatography facilities as alternative methods to purify target compounds.

- **Risk 2:** Synthesize large quantities (> 5L) of POMEs for engine testing

  Implications: Time consuming/expensive processes to synthesize POMEs from M-n-M and its corresponding alcohol (reaction, separation and purification)

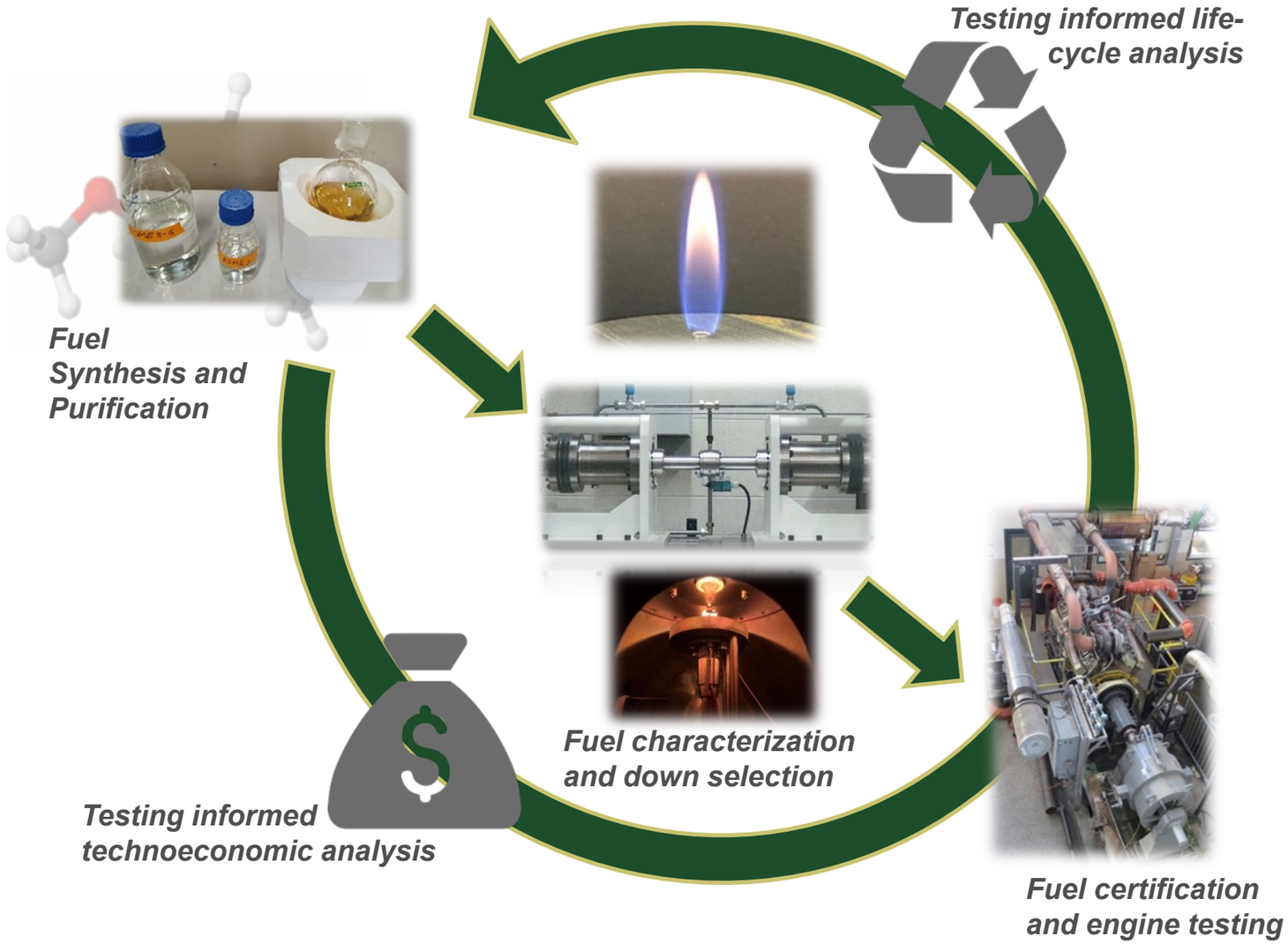
  Mitigation: Exploring multiple synthesis routes including route from commercially available dialkoxy-methane (e.g., B-1-B, P-1-P, etc.) with high product yields

- **Risk 3:** Synthesis of fuel from biomass

  Implications: Important to ensue product specifications and ensure no impact from impurities resulting from bio-processing

  Mitigation: We have identified bio-derived alcohol reactants for use in synthesis

2- Approach - Project



2- Approach – Project Flowchart

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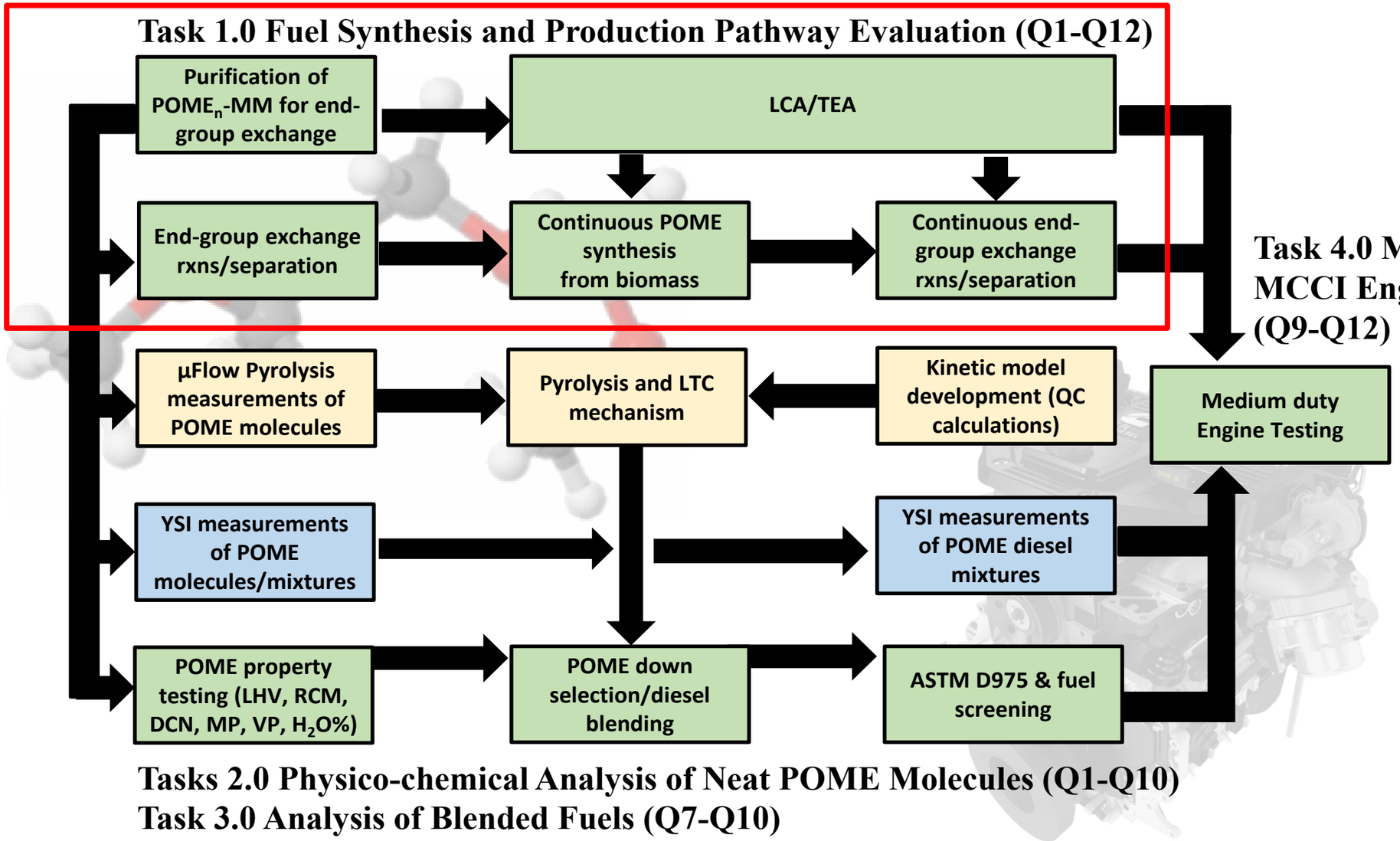


2 – Approach - Fuel Synthesis

Task 1.0 Fuel Synthesis and Production Pathway Evaluation

Dr. Kenneth Reardon

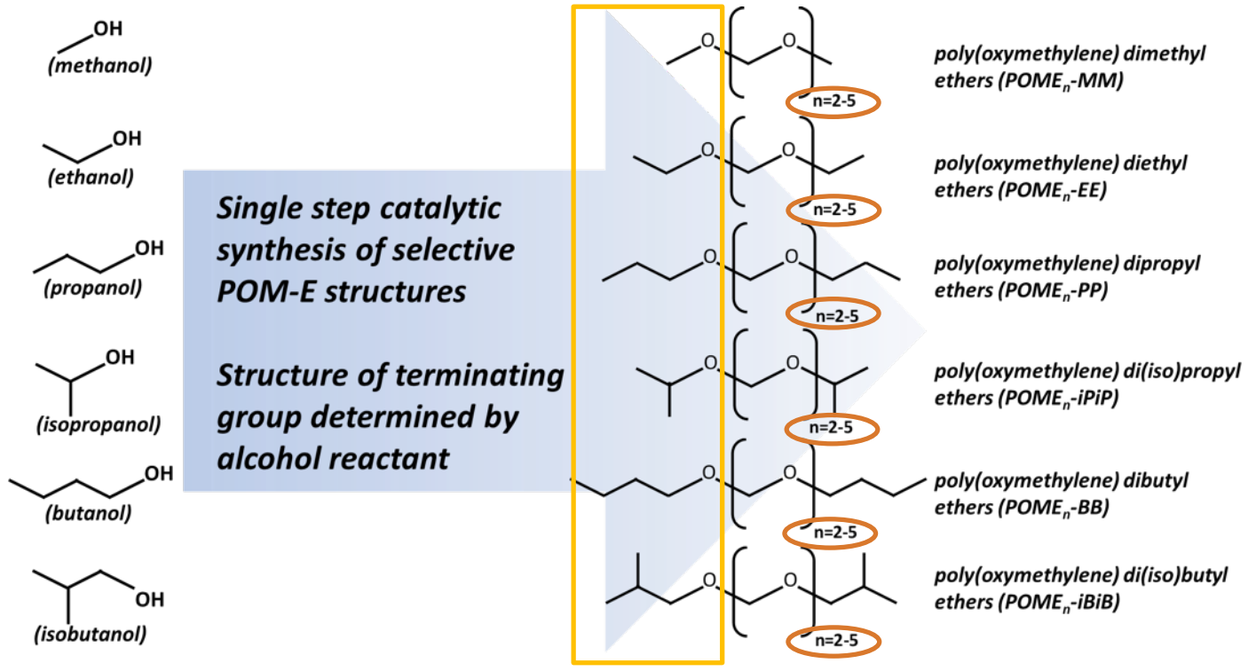
Dr. Thomas Foust

Dr. Jason Quinn

Goals

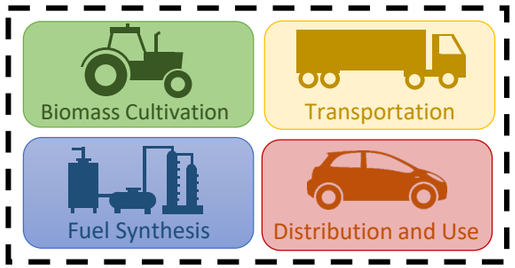
- Purchase, purification and upgrade of bulk M-n-M materials for initial optimization studies of POME structures
- Production of POME from lignocellulosic biomass as the feedstock material
- Rigorous TEA/ sustainability analysis to quantify expected GHG reduction from the produced POME advanced biofuels.

Approach

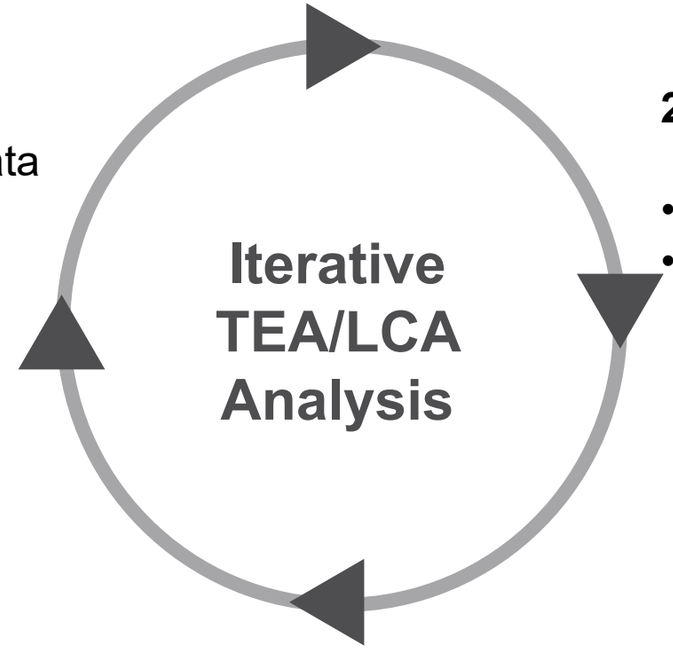


n = number of oxymethylene units, e.g., $(CH_2O)_n$
M,E,P,B – end alkyl group

2- Approach – Sustainability Assessment

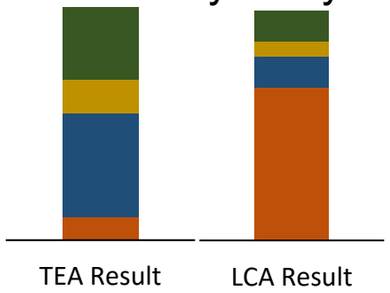


1. Process model
- Collect existing experimental data
- Supplement with literature data
- Quantify energy and materials

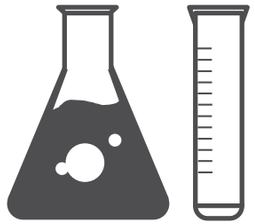


2. Life Cycle Assessment (LCA) & Techno-Economic Analysis (TEA)
- Quantify emissions (GHG, soot, other)
- Quantify minimum fuel selling price

3. Data Feedback & Validation
- Compare to other fuels/feedstocks
- Identify “hot-spots”
- Run uncertainty analyses



4. Experimental systems
- Define additional experiments
- Generate new data



2 – Approach - Project Flowchart

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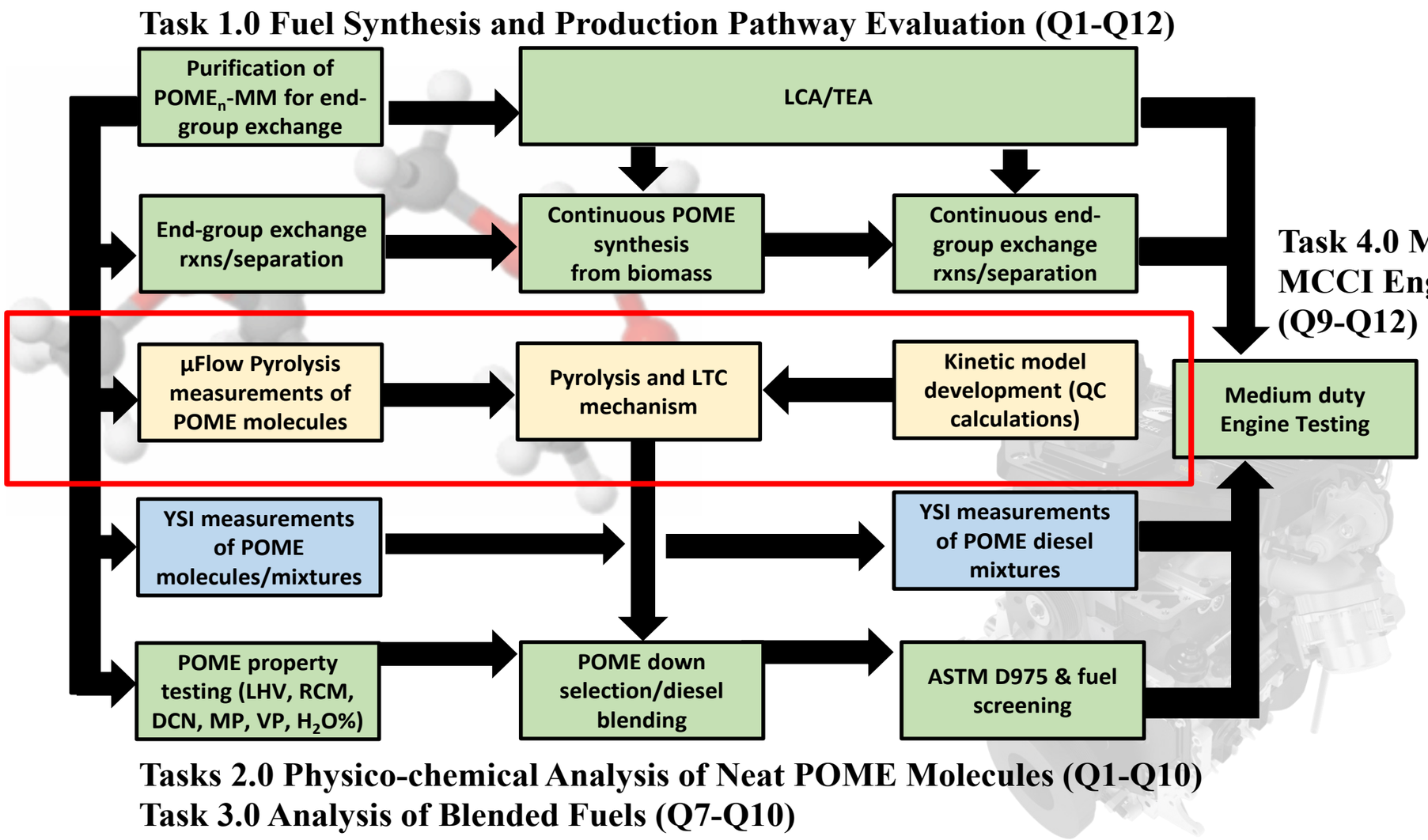
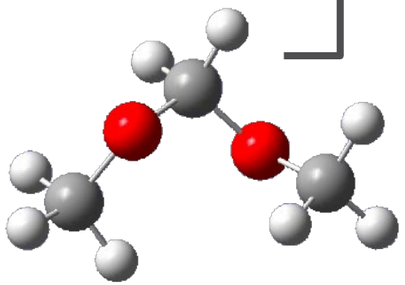


2- Approach – POME Reaction Pathways

Dr. Nicole Labbe

- **Subtask 2.1: Fundamental Chemistry Experiments Using μR-PIMS (Q1-Q8)**
  - Using a combined theory and experimental approach, our goal is to understand the kinetics of POMEs, which is critical for the implementation of POMEs as blendstocks for MCCI applications.
  - CU Boulder's contributions aim to provide molecular insight into the kinetic behavior of various POM-E structures and to provide kinetic sub-mechanisms to aid the fuel down selection and model their behavior in engines.

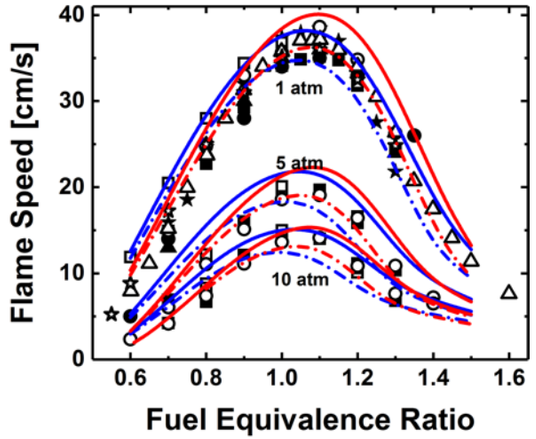
Micro-reactor PIMS Experiments



Electronic Structure Theory

Chemical Kinetic Mechanisms

Combustion Behavior Predictions



2 – Approach - Project Flowchart

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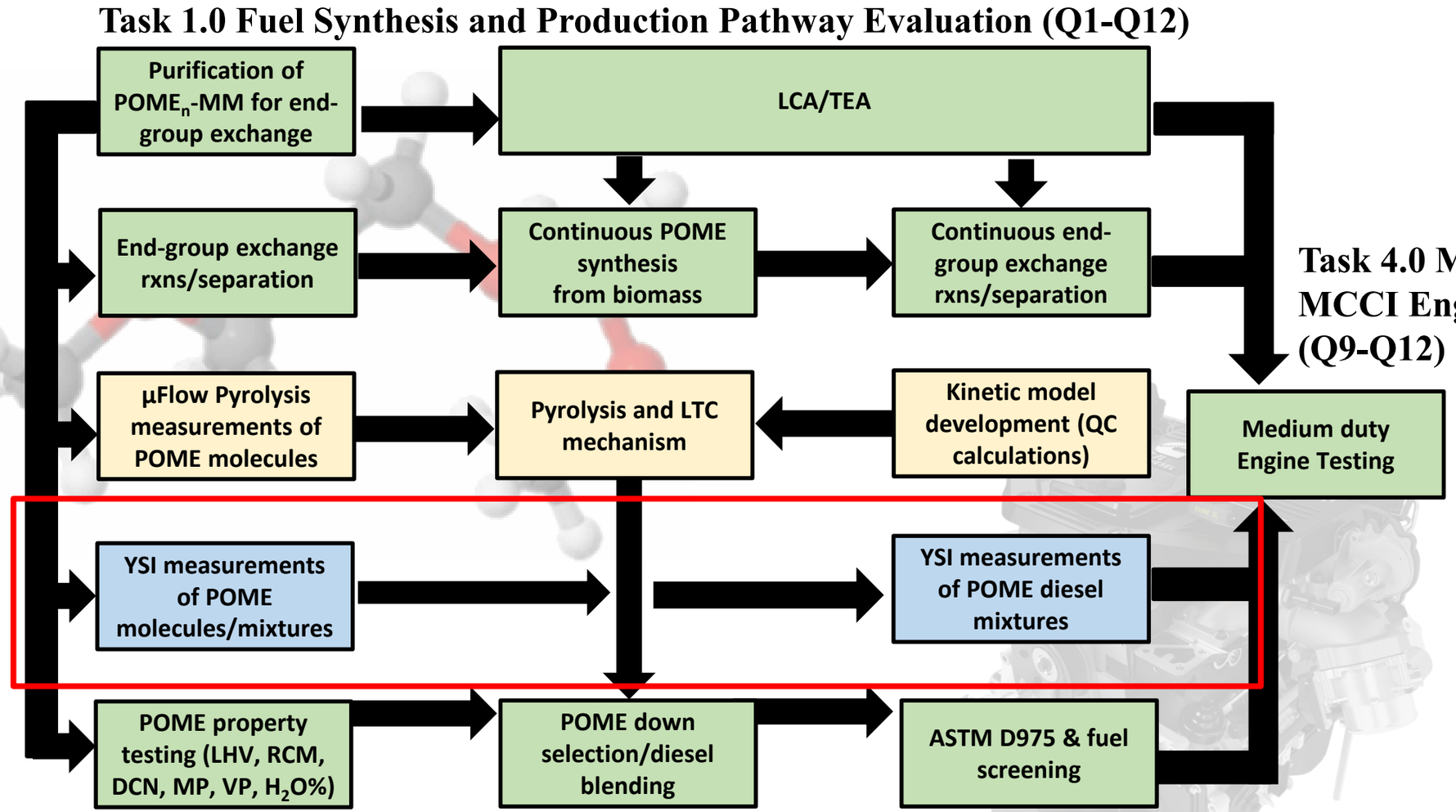


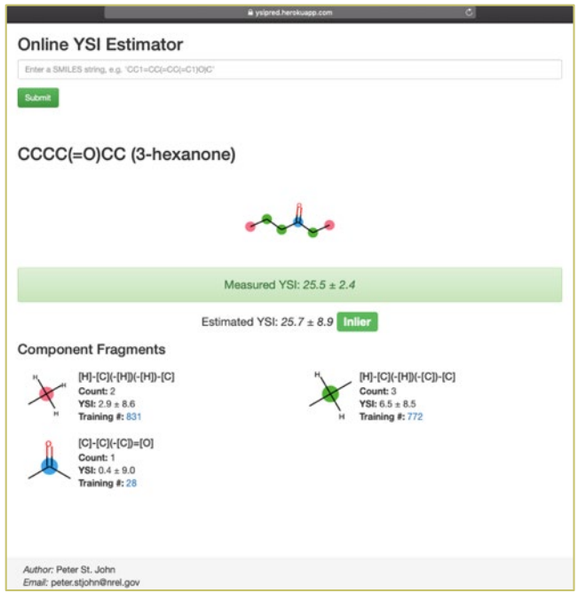
2 – Approach - POME Sooting Tendencies

Dr. Lisa Pfefferle

Dr. Charles McEnally

- **Subtask 2.3: Determine Sooting Tendencies of POME**

- Measure quantitative sooting tendencies of individual POMEs using the yield sooting index (YSI) metric
- Include target POMEs with a variety of end-groups (methyl, ethyl, propyl, butyl) and different numbers of oxymethylene units (1 to 5)
- Demonstrate that POMEs offer lower sooting tendencies than conventional diesel fuels
- Develop structure-property relationships that can predict YSI for arbitrary POME structures
- Use these relationships to optimize the trade-offs between sooting tendency and other fuel properties
- Make the POME structure-property relationships for sooting tendency available to all stakeholders via the NREL YSI estimation webapp



https://ysi.ml.nrel.gov

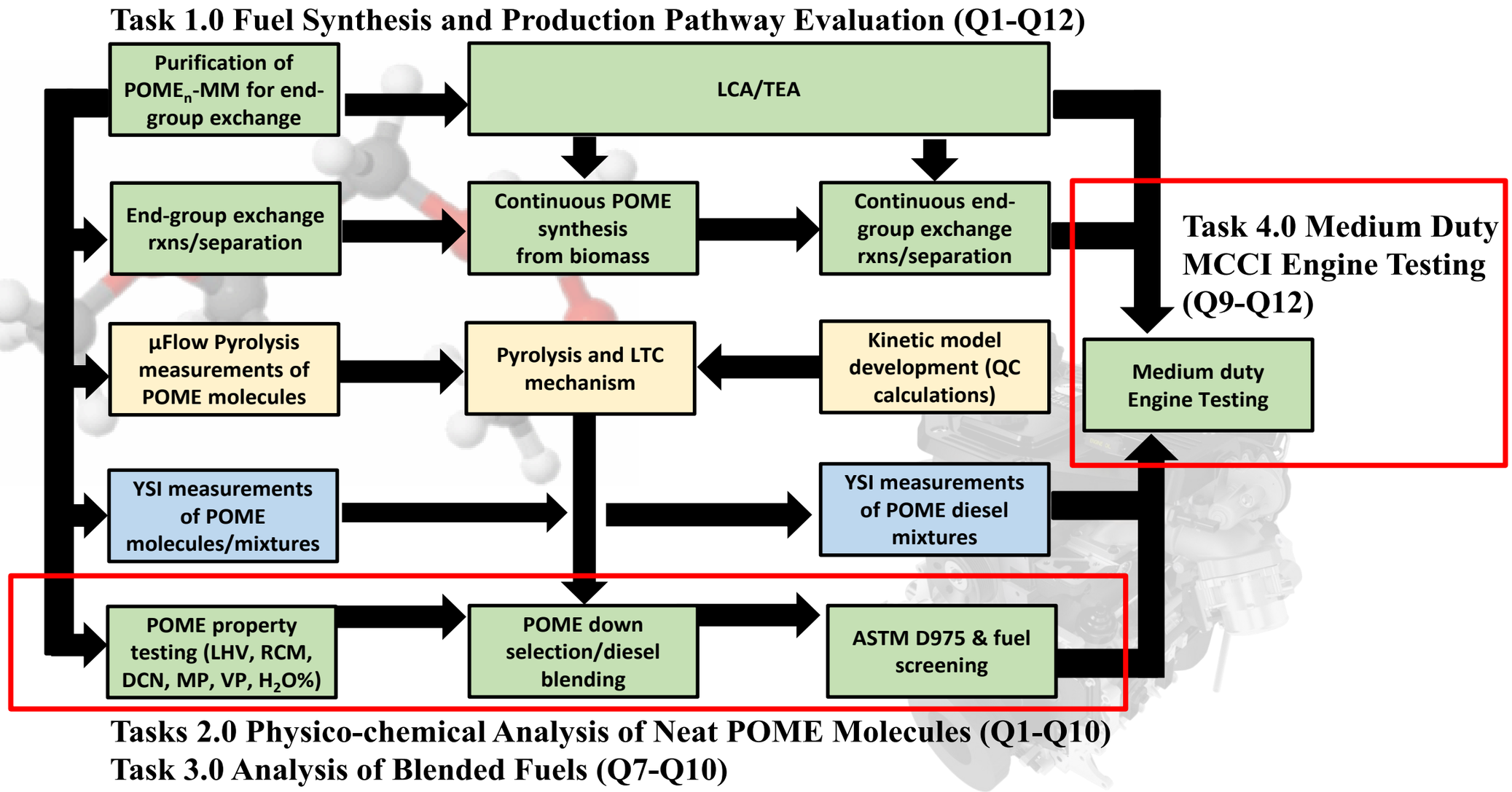
DBE: double bond equivalent
PM: particulate matter index

2 – Approach - Project Flowchart

CSU

CU-Boulder

Yale

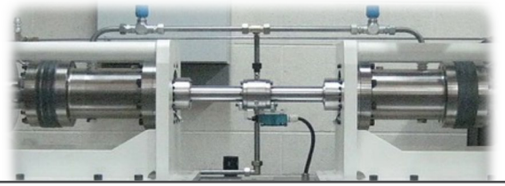


2 – Approach - POME Properties

Dr. Anthony Marchese

Task 2.0 Physico-chemical Analysis of Neat POME Molecules

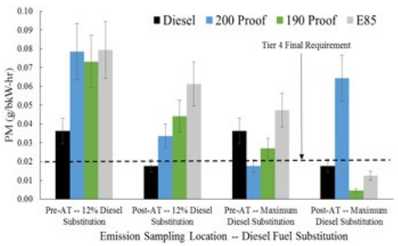
- **Subtask 2.5: Ignition Delay Measurement (RCM)**
  - *Using the RCM, homogeneous autoignition delays will be measured to determine the effect of POME structure on autoignition.*
- **Subtask 2.6: Fuel Stability/LHV Analysis**
  - *Melting/cloud points, cold flow plug points, water solubility, oxidative stability and LHV will be measured for the POME compounds/mixtures.*
- **Task 4.0 Medium Duty MCCI Engine Testing**
  - *Final fuel evaluation will be performed by way of engine testing in a Cummins 6.7L medium duty MCCI engine at the CSU Powerhouse.*
  - *High speed combustion, fuel consumption, and emissions (PM mass/number, 5-gas, and HC speciation) data*



Rapid Compression Machine

IKA C200 combustion calorimeter

Metrohm 743 Rancimet



Cummins 6.7L QSB Tier 4 Final engine test cell (left). Pre and post catalyst PM10 emissions for ethanol-diesel fuel blends.

2 – Approach – Go/No Go

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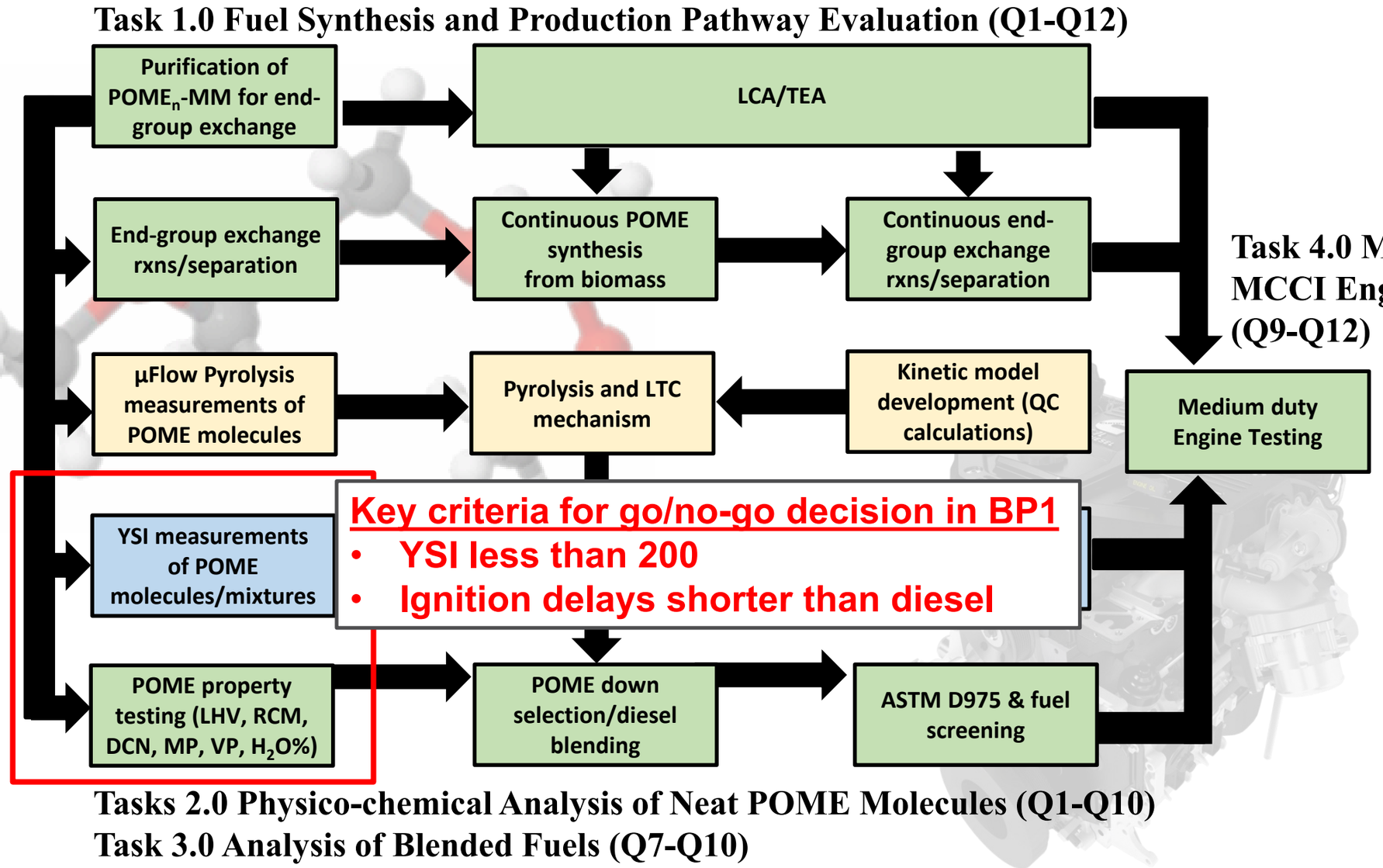
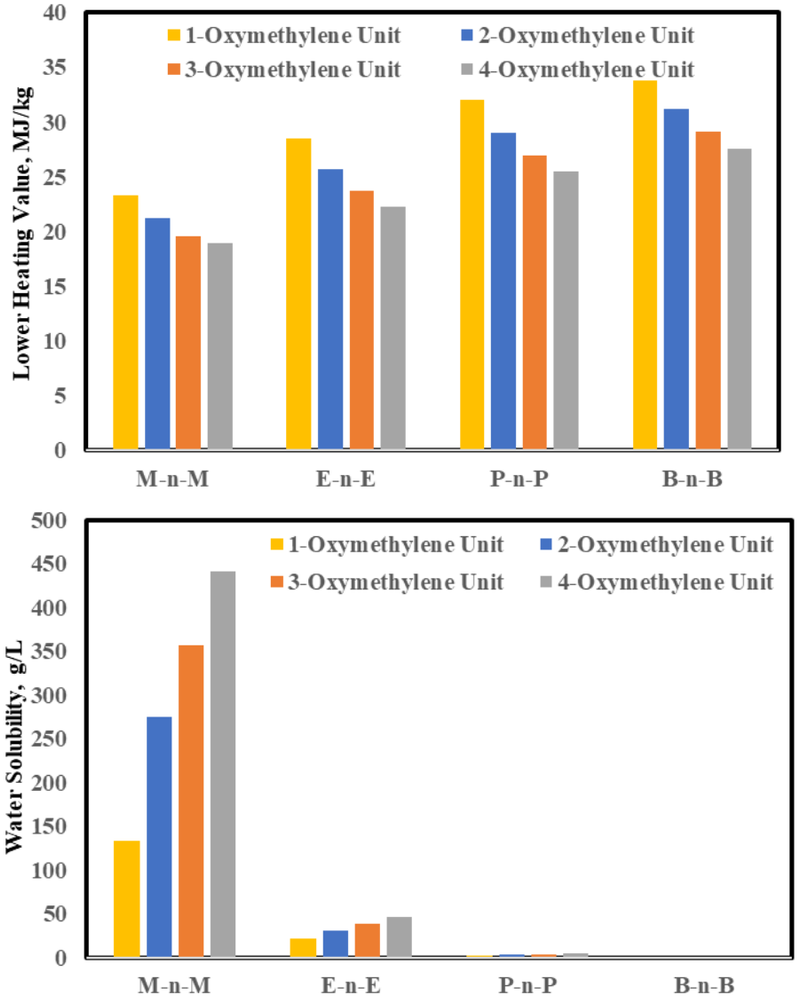


3- Impact – Improved Fuel Properties

- First to comprehensively investigate ***POMEs*** with C_2-C_4 end groups as bio-blendstocks
- High level characterization of the POME fuels allows engine co-development to maximize energy conversion efficiencies and minimize pollutant formation in MCCI engine platforms.
- Modelling results revealed that these novel POMEs exhibit **favorable physico-chemical properties** required by a diesel blendstock while still exhibiting remarkable soot reduction potential.
- Identify viable low-carbon footprint and cost-effective production pathways for POME needed for scale-up.

Structure-activity model predictions



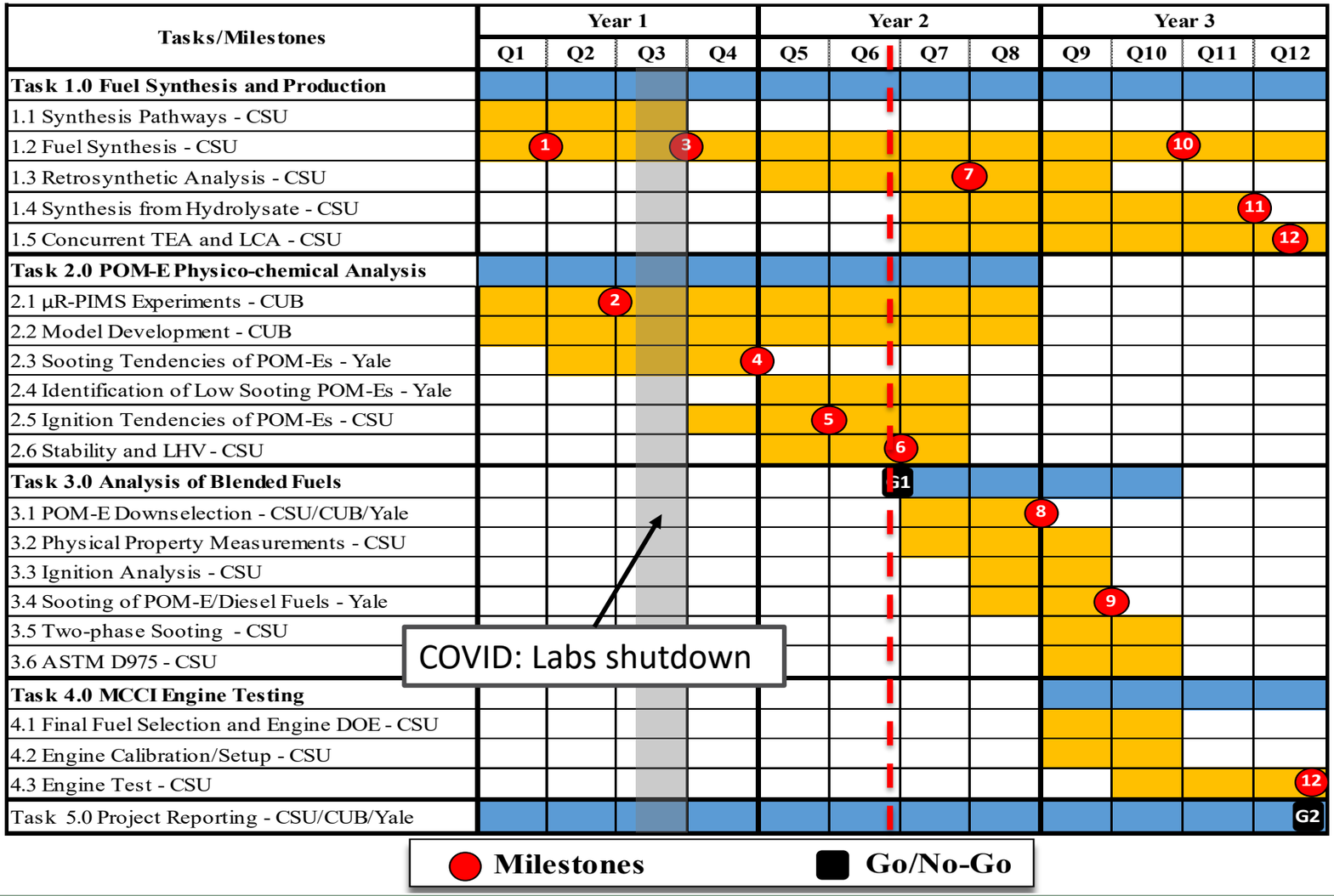
Work recently accepted for publication: Bartholet, D., et al., "Property predictions of structurally diverse polyoxymethylene ethers as potential diesel blendstocks." **Fuel, 2021**, Manuscript accepted. **Impact factor- 5.578**

3- Impact

- Research outputs will be published in **High Impact Factor Journals,** including:

1. Bartholet, D., et al., "Property predictions of structurally diverse polyoxymethylene ethers as potential diesel blendstocks." **Fuel, 2021**, Manuscript accepted. **Impact factor- 5.578**
2. Arellano-Treviño, M.A. et al., "Synthesis of butyl-exchanged polyoxymethylene ethers as renewable diesel blendstocks with improved fuel properties" Manuscript submitted to ACS Sustainable Chemistry & Engineering Journal. **Impact factor- 7.632**
3. Zhu, J., et al., "Sooting tendencies of individual polyoxymethylene ethers with methyl, ethyl, propyl, and butyl end-groups and one to five oxymethylene units", Manuscript in preparation, **Applications in Energy and Combustion Science.**
4. Chan, F.L., et al., "Recent developments on polyoxymethylene dimethyl ether as a renewable diesel fuel blendstock**"**, Proposal submitted to **Chemical Reviews. Impact Factor- 52.758**
5. Chan, F.L., et al., "Cation Exchange Resins Catalyzed Synthesis of Dibutoxymethane: a diesel fuel blendstock for Soot Reduction", Manuscript in preparation, **Fuel Processing Technologies. Impact Factor- 4.982**
6. Sampathkumar, J. et al., "Chain length effects on the thermal decomposition of polyoxymethylene ethers," Manuscript in preparation. Combustion and Flame. **Impact factor- 4.570**
7. Aguirre et al., "Structural effects of methyl, ethyl and propyl end groups on the pyrolysis of polyoxymethylene ethers ," Manuscript in preparation. Combustion and Flame. **Impact factor- 4.570**

4- Progress and Outcomes



4- Progress and Outcomes

Milestone 1.2.1 (Q1): Purchase and purification of more than 50 mL of M-n-M oligomers for subsequent testing with documented production pathways from lignocellulosic biomass

Milestone 2.1 (Q2): Measure species profiles identifying pyrolysis pathways for M-n-M oligomers

Milestone 1.2.2 (Q3): Production of more than 10 mL of POME with alkyl group of C2 or greater for subsequent testing with documented production pathways from lignocellulosic biomass

Milestone 2.4 (Q4): Post at least 10 new YSIs measured for POME and related compounds to the online YSI database.

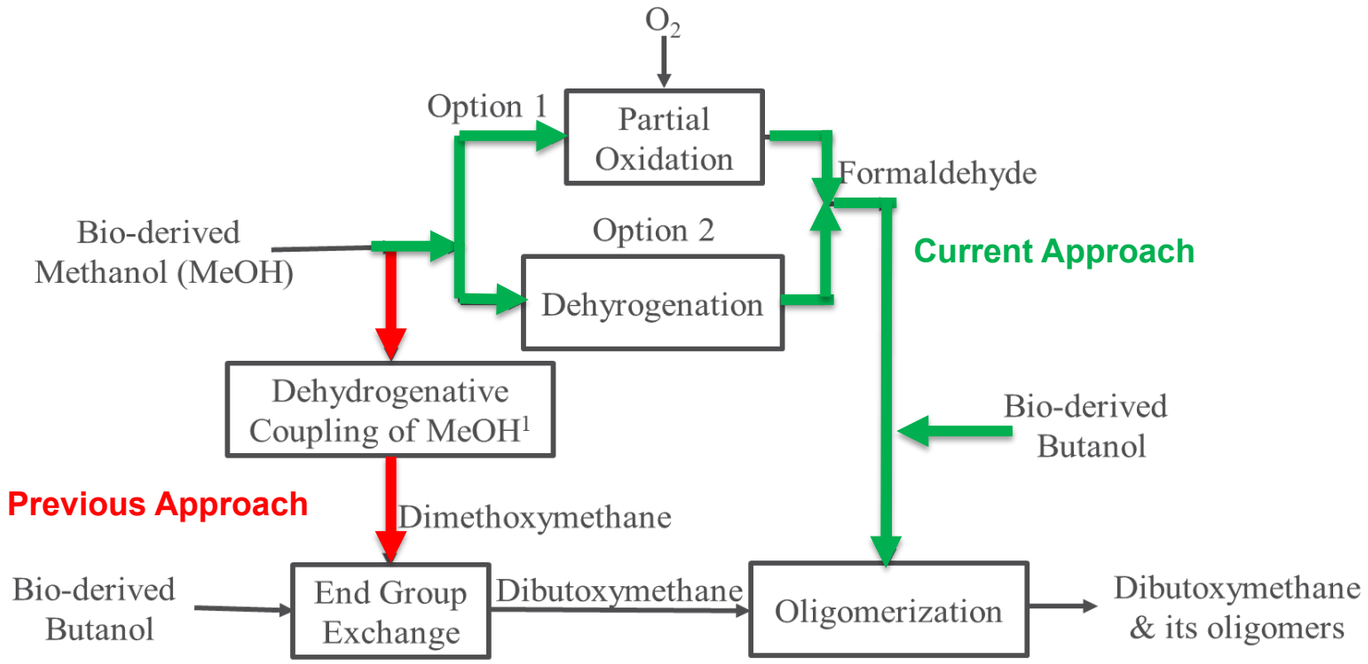
Milestone 2.5 (Q5): Gas phase ignition characterization of at least 10 POME and related compounds with empirical trend correlating POME polymerization and terminating group to gas phase ignition delay

Milestone 2.6 (Q6): Oxidative stability and LHV measurements of at least 10 POME and related compounds with empirical trend linking POME polymerization and terminating group to oxidative stability and LHV

4- Progress and Outcomes - Synthesis

Task 1.0- Fuel Synthesis and Production

Current approach for the synthesis of butyl terminated POMEs



Product Yields Comparison

	Previous Approach	Current Approach
B-1-B	14 %	**55 %**
B-2-B	4 %	**24 %**
B-3-B	1 %	**11 %**

- **Limited POME yield in original synthesis approach**
- **New approach will generate greater yield including larger (n > 2) POME oligomers!**

[1] To, A.T., et al., Dehydrogenative Coupling of Methanol for the Gas-Phase, One-Step Synthesis of Dimethoxymethane over Supported Copper Catalysts. ACS Sustainable Chemistry & Engineering, 2020. 8(32): p. 12151-12160.

4- Progress and Outcomes - Synthesis

Milestone 1.2.2 (Q3): Production of more than 10 mL of POMEs with alkyl group of C2 or greater for subsequent testing with documented production pathways from lignocellulosic biomass

Current POME Inventory

Compound	Quantity (ml)
B-1-B	> 500
B-2-B	91
B-3-B	25
P-1-P	> 500
P-2-P	40
P-3-P	25
E-1-E	> 500
E-2-E	40
E-3-E	25

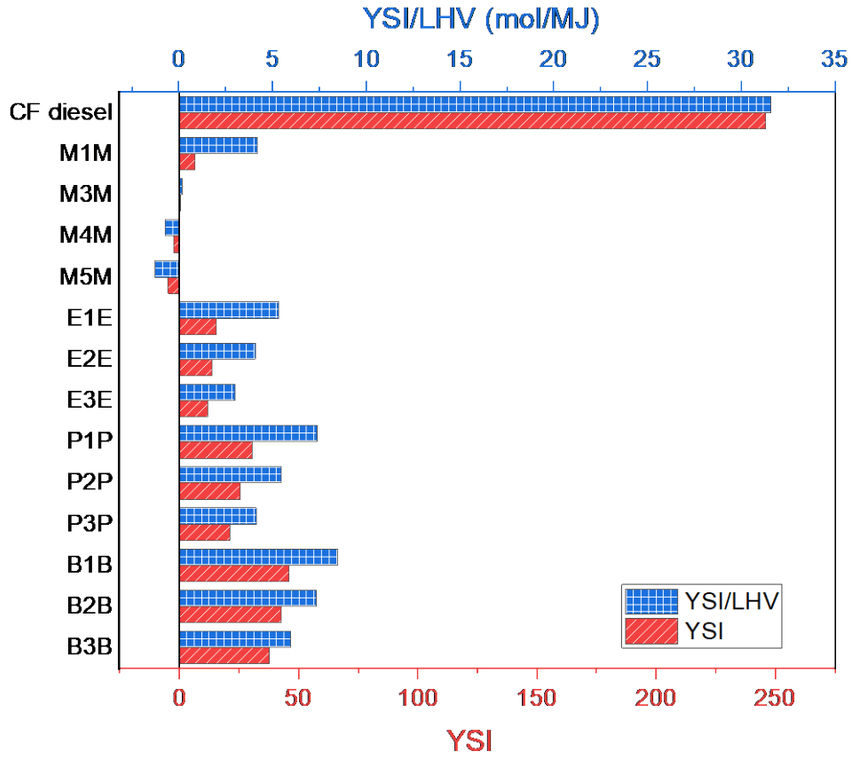
Able to selectively synthesize necessary volumes of POME with varying end groups and oxymethylene units for subsequent testing!

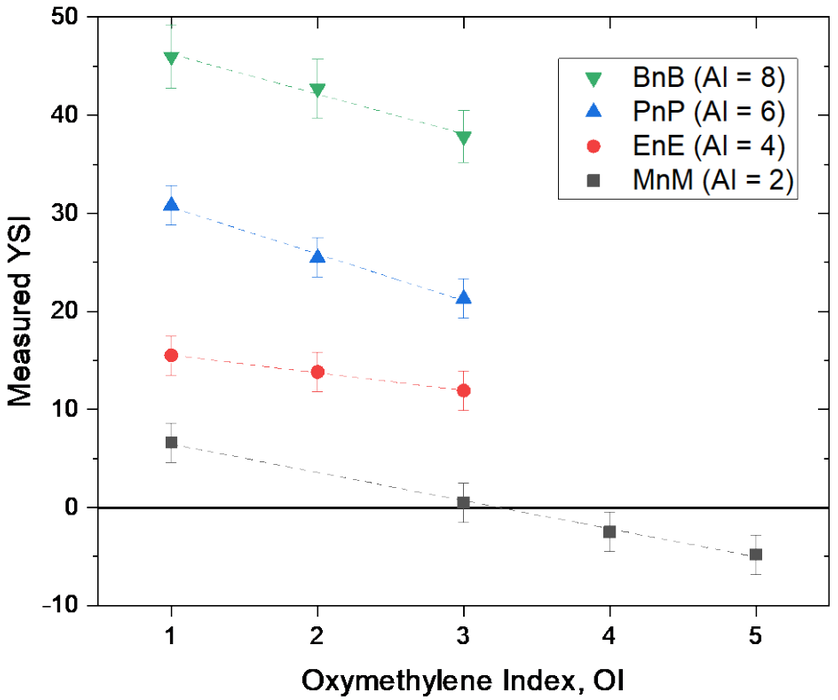
4- Progress and Outcomes - YSI

Task 2.0- POMEs physico-chemical analysis
Milestone 2.4 (Q4): Post 10 new YSIs measured for POME and related compounds to the online YSI database.

Sooting tendencies of POMEs

- Sooting tendencies (YSIs) were measured for 13 individual POMEs synthesized and purified at Colorado State University
- The YSIs have been posted to the Github page that is used as training data for the NREL YSI estimation tool (https://ysi.ml.nrel.gov)
- This data can be used to rationally select POME structures that optimize the trade-offs between fuel properties





All of the POMEs sooted much less than a certification diesel fuel

Work Submitted: Zhu, J., et al., "Sooting tendencies of individual polyoxymethylene ethers with methyl, ethyl, propyl, and butyl end-groups and one to five oxymethylene units", Manuscript in preparation, **Applications in Energy and Combustion Science.**

4 - Progress and Outcomes - YSI

Task 2.0- POMEs physico-chemical analysis

YSI of POMEs

- The measured YSIs can be fit to within ±1.6 YSI units with the empirical correlation:

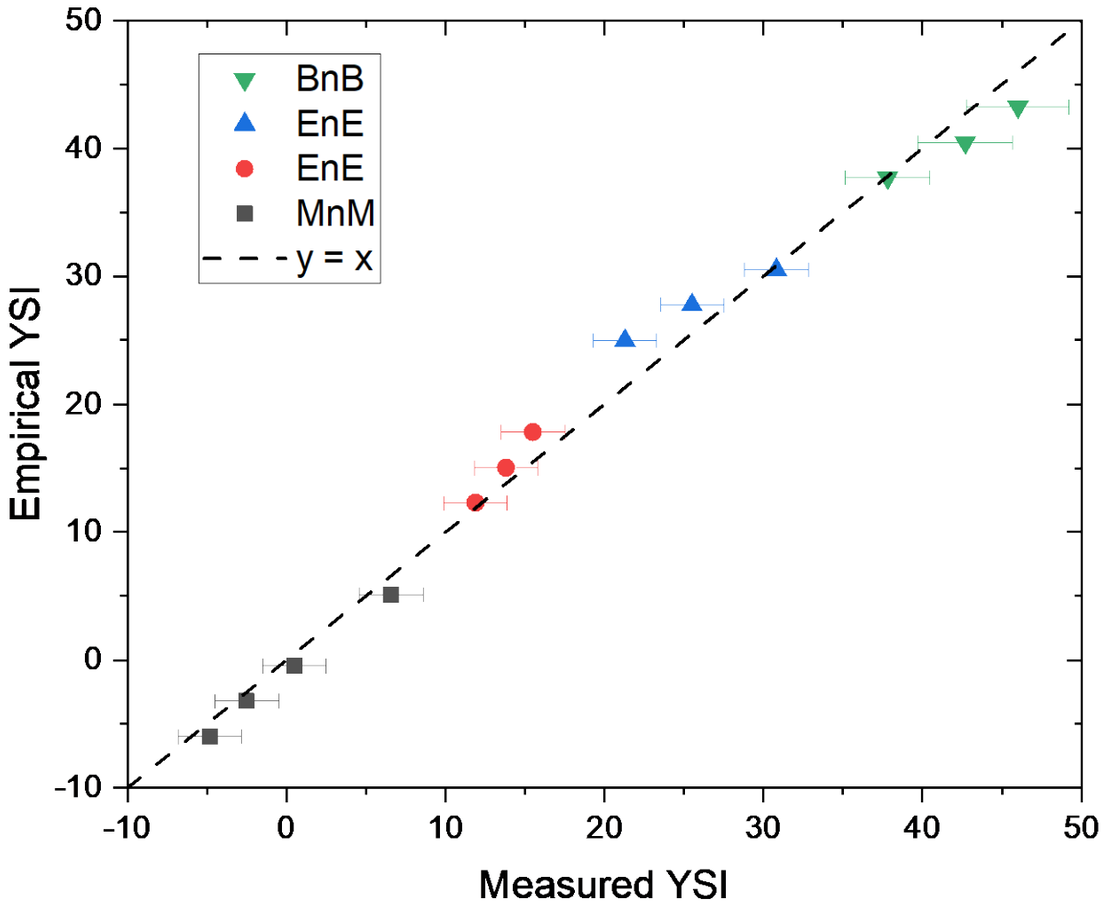
$$YSI = 6.359 \times \mathbf{AI} - 2.768 \times \mathbf{OI} - 4.869$$

- AI and OI represent Alkyl index and Oxymethylene Index
- Simplified reaction pathways show that the trends in YSI can be explained in terms of pyrolysis products
- This reaction pathway analysis can be extended to estimate YSIs for POMEs that have not yet been synthesized

$$POME \rightarrow (OI+1)CH_2O + H + CH_3 + (AI/2-1)C_2H_4$$

diluents that suppress soot

hydrocarbons that enhance soot

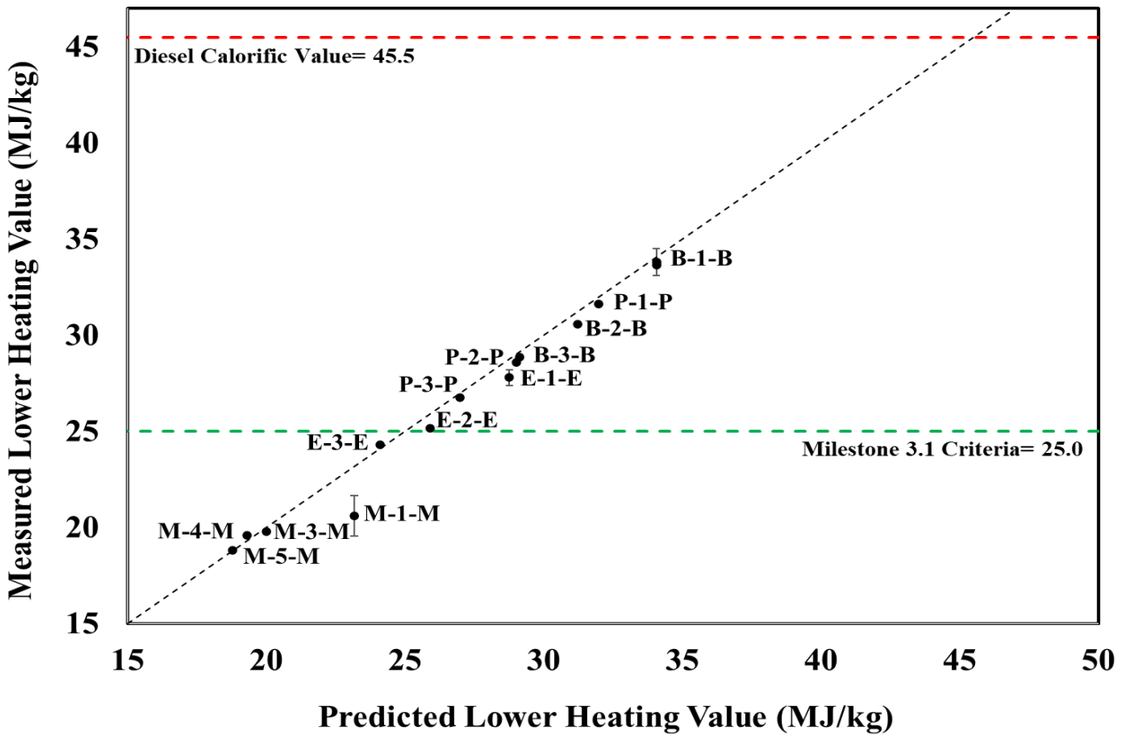


Can correlate POME sooting tendency to end-group length and number of oxymethylene units

4- Progress and Outcomes – Properties

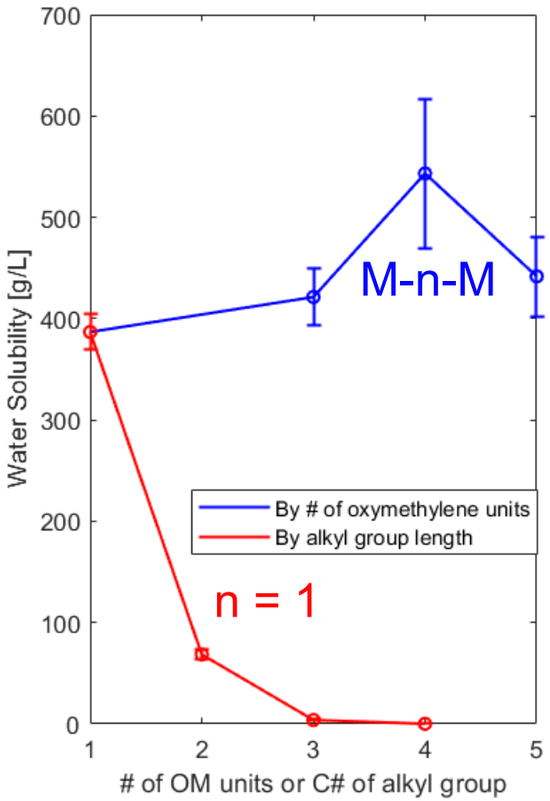
Task 2.0- POMEs physico-chemical analysis

Lower Heating Values of POMEs



- **Larger end groups increase LHV!**

Water Solubility of POMES

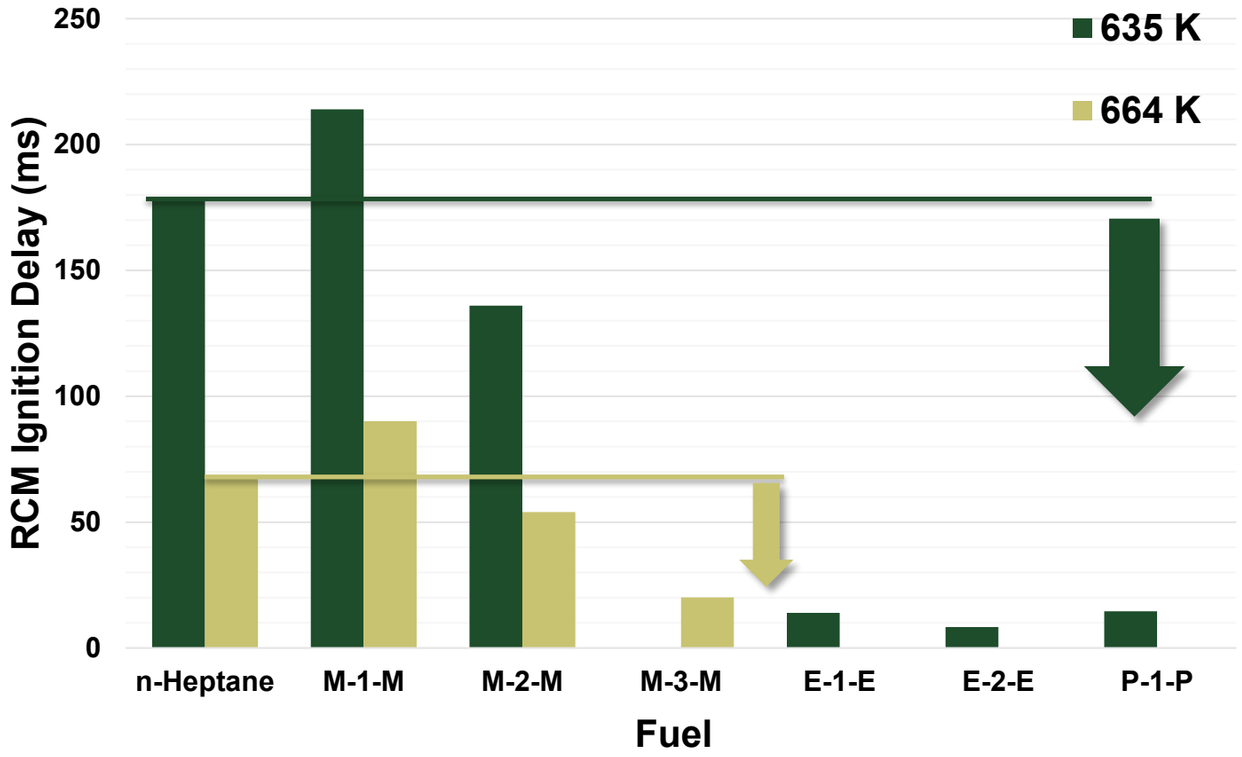


- **Larger end groups significantly reduce water solubility**

4- Progress and Outcomes - Ignition

Task 2.0- POMEs physico-chemical analysis

Gas-Phase Ignition Delay.



- **Larger end groups and increased number of oxymethylene units result in faster autoignition than diesel (n-heptane)**

4- Progress and Outcomes - Kinetics

Subtask 2.1 & 2.2: µR-PIMS Experiments and Theory-based predictive modeling

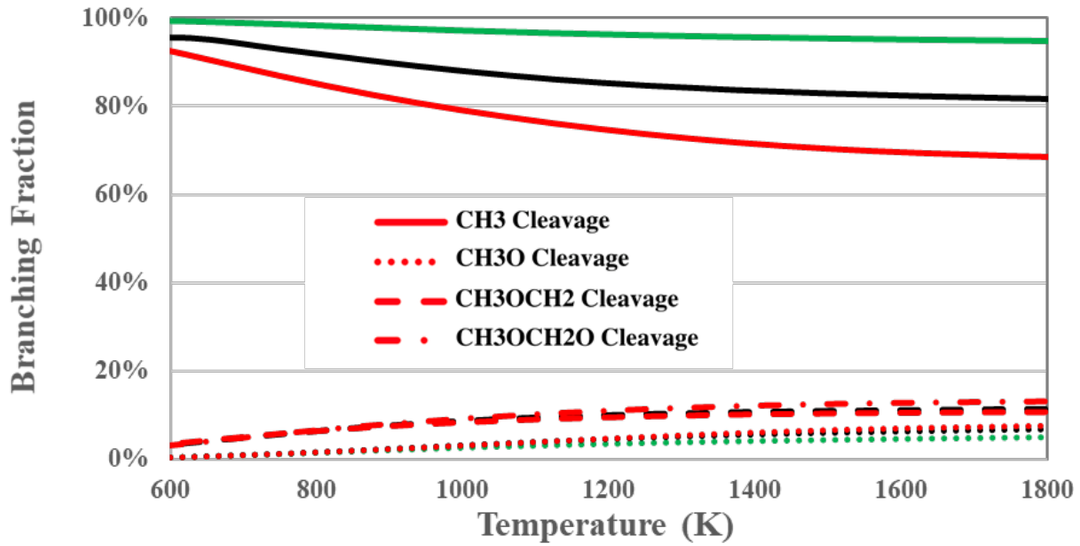
Purpose:

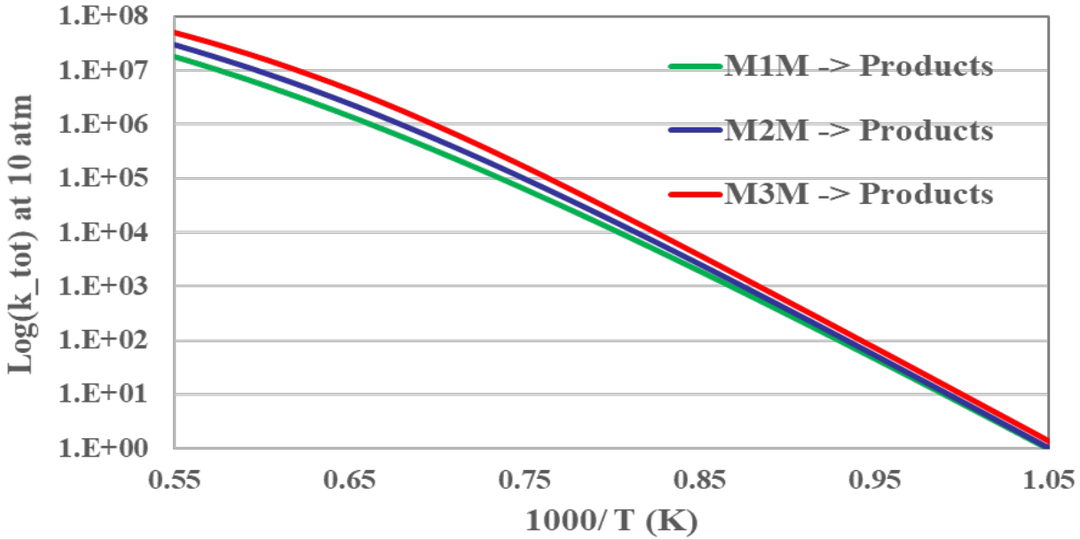
- Identify how chemical structure influence reaction properties for various POMEs.
- Provide detailed chemical models to predict combustion behaviors at engine relevant temperatures and pressures (Chemkin models).

Initial Results:

- CH_3 cleavage dominates reaction for all M-n-Ms and confirmed by µR-PIMS Experiments (top)
- Overall reaction rate increases with M-n-M chain length (bottom)

- **Reaction results support YSI and Ignition measurement trends: increased chain length increases early time scale dilution (lowers YSI) and enhanced POME reactivity (lower ignition delay).**





Summary

- Achieved all the milestones proposed for the FY20 and first half of FY21.
- Novel POMEs exhibit favorable physicochemical properties required by a diesel blendstock (**higher LHV, lower water solubility)** while still exhibiting **remarkable soot reduction potential and faster ignition chemistry than diesel fuel**.
  - Sooting tendencies (YSIs) of POMEs were less than 25% that of certified diesel fuel.
  - YSIs of POMEs can be accurately predicted with the empirical formula within ±1.6 YSI units.
  - All POMEs, except the dimethoxymethane (M-1-M), exhibited shorter ignition delay compares to diesel surrogate heptane.
  - Results from M-1-M pyrolysis study revealed that bond fission and rapid dissociation are the dominant reactions that produce methyl and formaldehyde radicals.
- Future work will investigate sustainability/economics and test the down selected blendstock performance in a medium duty diesel engine

Thank you

This material is based upon work supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (EERE) under the Bioenergy Technologies Office, Co-Optimization of Fuels and Engines Initiative award number DE-EE0008726. Authors acknowledge additional financial support from the Colorado Energy Research Collaboratory (Collaboratory).

Colorado State University

Colorado Energy Research Collaboratory
Securing a Sustainable & Resilient Energy Future

U.S. DEPARTMENT OF ENERGY

Publications

Journal Publications Submitted/Prepared

1. Bartholet, D., et al., "Property predictions of structurally diverse polyoxymethylene ethers as potential diesel blendstocks." **Fuel, 2021**, Manuscript accepted. **Impact factor- 5.578**
2. Arellano-Treviño, M.A. et al., "Synthesis of butyl-exchanged polyoxymethylene ethers as renewable diesel blendstocks with improved fuel properties" Manuscript submitted to ACS Sustainable Chemistry & Engineering Journal. **Impact factor- 7.632**
3. Zhu, J., et al., "Sooting tendencies of individual polyoxymethylene ethers with methyl, ethyl, propyl, and butyl end-groups and one to five oxymethylene units", Manuscript in preparation, **Applications in Energy and Combustion Science.**
4. Chan, F.L., et al., "Recent developments on polyoxymethylene dimethyl ether as a renewable diesel fuel blendstock**"**, Proposal submitted to **Chemical Reviews. Impact Factor- 52.758**
5. Chan, F.L., et al., "Cation Exchange Resins Catalyzed Synthesis of Dibutoxymethane: a diesel fuel blendstock for Soot Reduction", Manuscript in preparation, **Fuel Processing Technologies. Impact Factor- 4.982**
6. Sampathkumar, J. et al., "Chain length effects on the thermal decomposition of polyoxymethylene ethers," Manuscript in preparation. Combustion and Flame. **Impact factor- 4.570**
7. Aguirre et al., "Structural effects of methyl, ethyl and propyl end groups on the pyrolysis of polyoxymethylene ethers ," Manuscript in preparation. Combustion and Flame. **Impact factor- 4.570**

Publications

Oral Presentations

1. Charles McEnally, “The effects of molecular structure on the sooting tendencies of fuels,” seminar presented at the National Renewable Energy Laboratory, Golden CO, 7 October 2019.
2. Charles McEnally, “YSI: a metric for assessing the soot-reducing potential of new fuel molecules,” seminar presented at Colorado State University, Fort Collins CO, 9 October 2019.
3. Bret Windom, "Poly(oxymethylene) Ethers (POM-E) as a High Cetane, Low Sooting Biofuel Blendstock for Use in MCCI Engines" presented at Co-optima Lighting Round, 9 January 2020.
4. Bret Windom, “Polyoxymethylene Ethers (POME) as a High Cetane, Low Sooting Biofuel Blendstock for Use in MCCI Engines”, Co-Optima All Hands Meeting, 2020.
5. Charles S. McEnally, “Background for soot metrics discussion,” presentation during the Co-optima Soot Discussion organized by the AED Team on 26 March 2020.
6. Junqing Zhu, “Poly(oxymethylene) Ethers: Potential Diesel Fuels with Low Sooting Tendencies,” AIChE Annual Meeting 2020, 17 November 2020.

Publications

Poster Presentation

1. Zhu, J., et al., “Poly(oxymethylene) Ethers (POMEs): potential diesel fuels with low sooting tendencies”, 38th International Symposium on Combustion, WIPP, LF-12, 24-29 January 2021.
2. Lucas, S., et al., “Polyoxymethylene ethers as low-sooting compression ignition fuels”, 38th International Symposium on Combustion, WIPP, ICE-05, 24-29 January 2021.

Upcoming Conference

1. Zhu, J. et al., “Low sooting tendencies of individual polyoxymethylene ethers as alternative diesel fuels”, ACS Spring 2021.
2. Chan, F.L. et al., “Extended alkyl terminated polyoxymethylene ethers as a potential renewable diesel fuel blendstock: synthesis approaches and physiochemical property characterization”, ACS Spring 2021.
3. Lockwood, K. et al., “A combined experimental and theoretical approach for understanding molecular structure effects on targeted fuel properties”, ACS Spring 2021.

Quad Chart

Timeline

- May 31, 2019
- September 1, 2022

	FY20 Costed	Total Award
DOE Funding	(9/01/2019 – 8/31/2022)	$1,972,050
Project Cost Share	(9/01/2019 – 8/31/2022)	$499,369

Project Partners

- University of Colorado - Boulder
- Yale University

Project Goal

The goal of the project is to identify the soot reduction potential, cetane number enhancement, and physico-chemical properties of poly(oxymethylene) ethers and identify an optimal biofuel blendstock comprised of POMEs that presents viable production pathways from lignocellulosic feedstocks and that enhances the performance and reduces criteria PM emissions of traditional MCCI fuels.

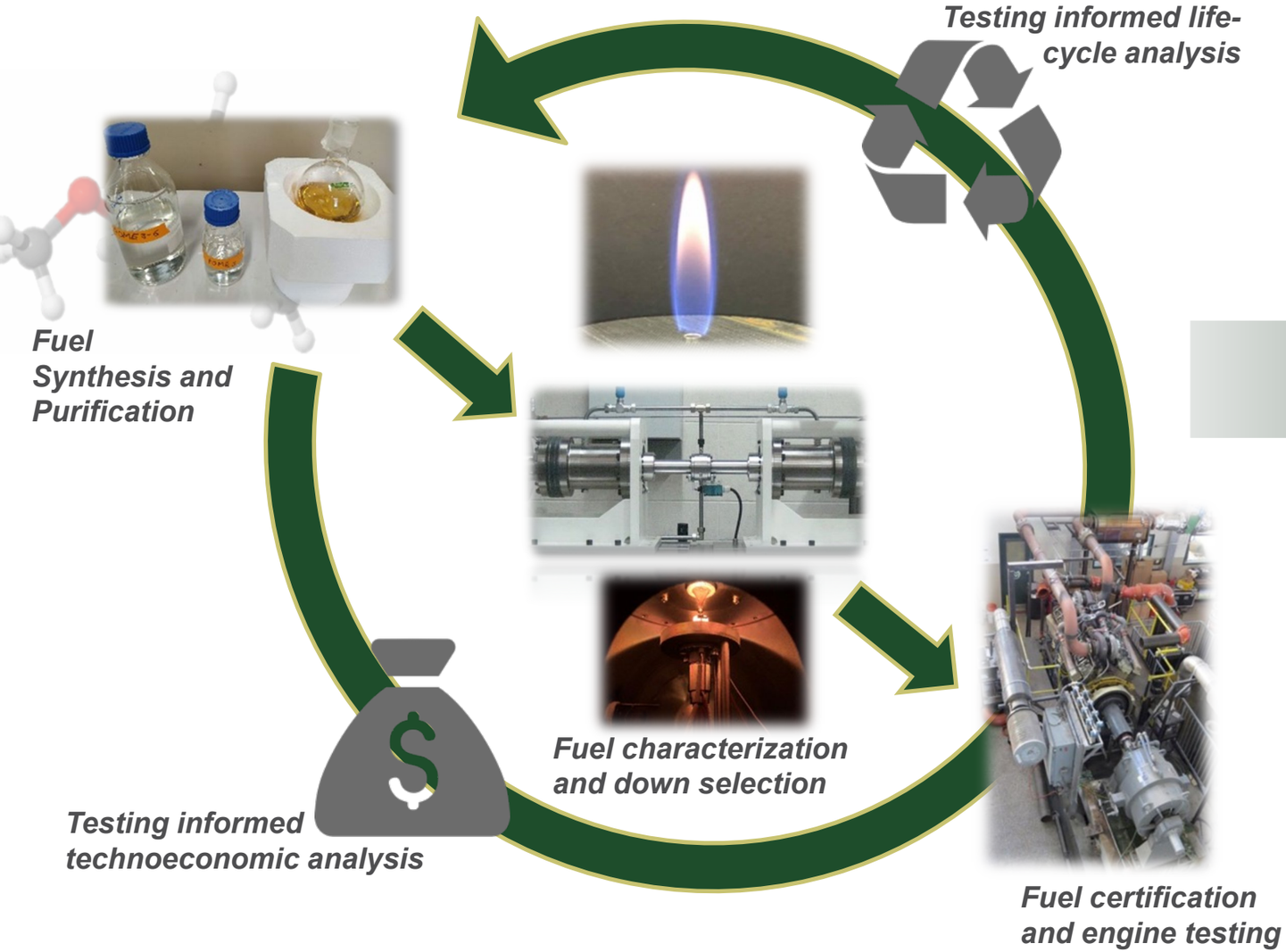
End of Project Milestone

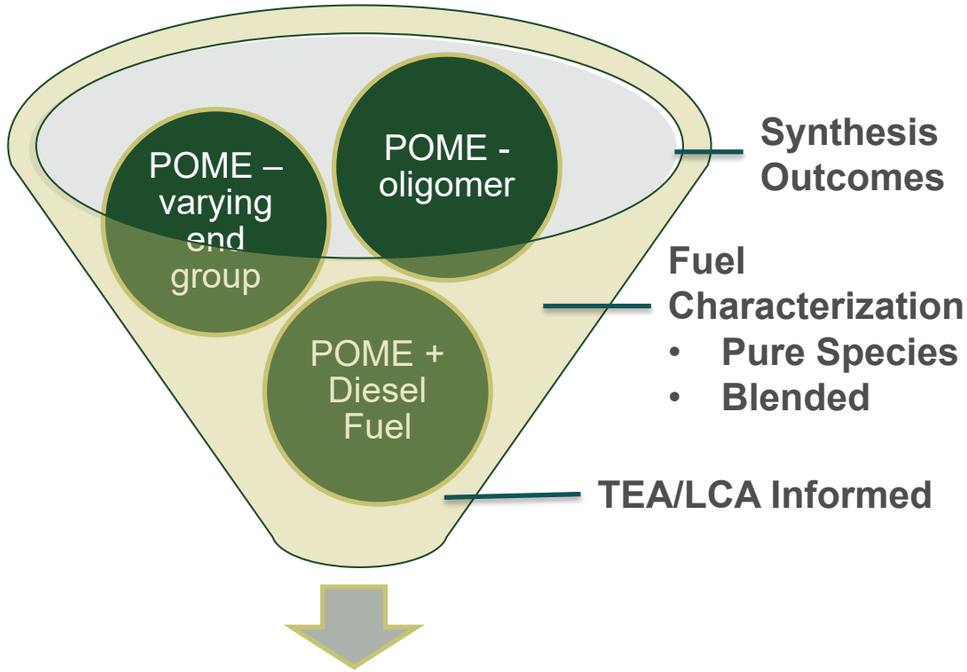
Production of at least 5 L of POM-E that exhibit acceptable DCN (greater than 40), YSI (less than 200), cold flow properties (melting points less than 0 C), and LHV (greater than 25 MJ/kg) along with engine testing with blended POM-E/diesel fuel (at least 5 vol% blending levels) with accompanying TEA/LCA to suggest optimal blends for scale up and commercialization.

Funding Mechanism

DE-FOA-0001919, Topic 5a - Multi-Mode Optimized Fuel/Engine System Development, 7/13/2018

Backup - Approach - Project

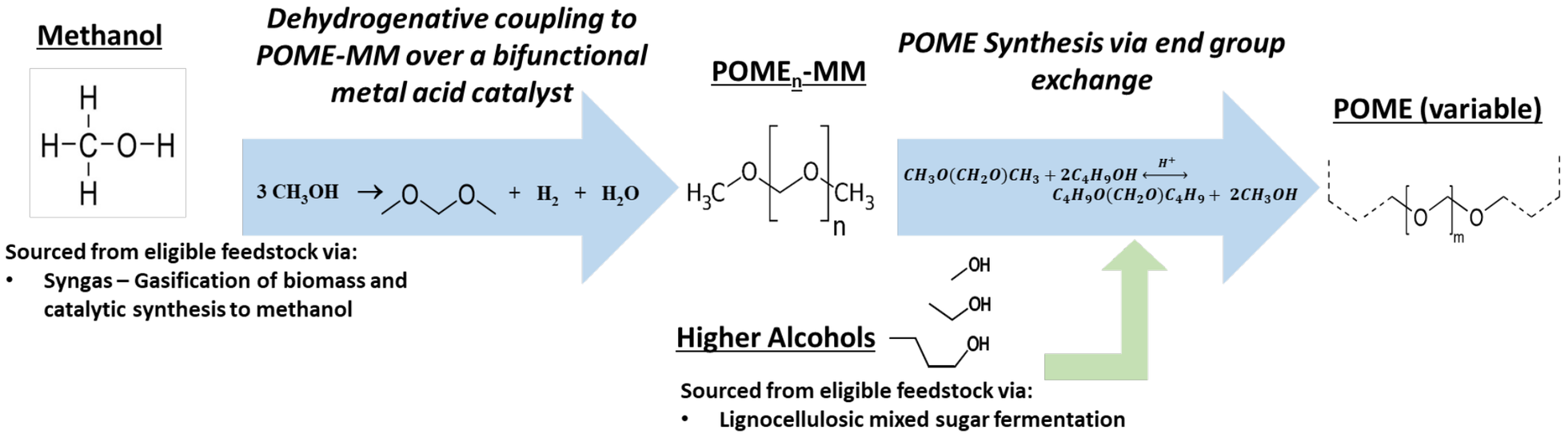




Optimized MCCI fuel composition and blend levels for use in ASTM D975 certification and engine testing.

Backup – Original Synthesis Approach

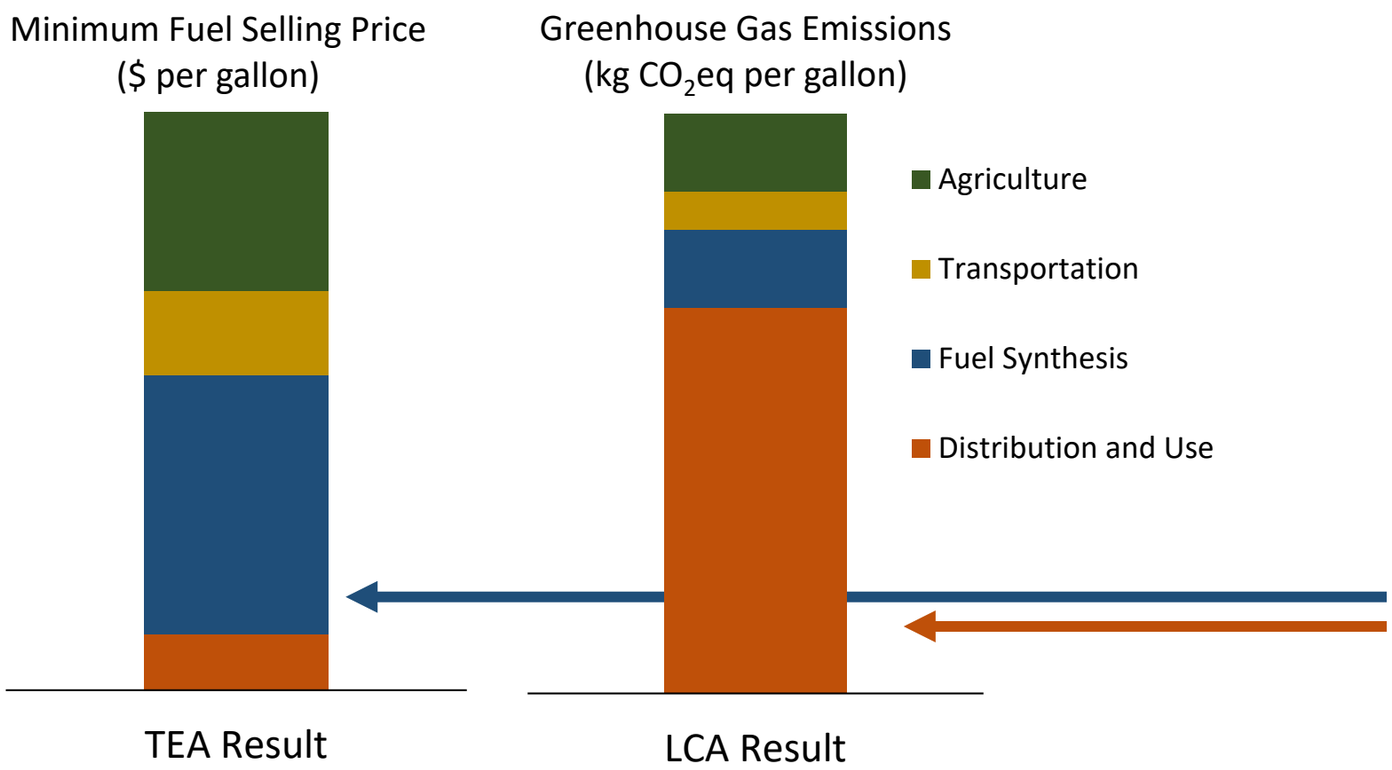
Proposed overall production approach from lignocellulosic feedstocks (Butyl terminated POMEs)



Challenges

- Low yields in first step – exploring alternative routes for POME-MM production via bio-methanol to formaldehyde
- In-house bio-formaldehyde production/sourcing
- Procurement of bio-derived large alcohols
- Increase level of difficulty in downstream separation process due to high number of by-products produced.

Backup - Impact – TEA/LCA



LCA and TEA will allow us to:

- Quantify environmental impact of POM-E
- Quantify economic costs of POM-E
- Compare with other fuels and blendstocks
- Inform future experiments and ongoing work
- Identify high impact “hot-spots”
- Advance existing life cycle inventory

Backup - Engine Demonstration

Task 4.0 Medium Duty MCCI Engine Testing

- Final fuel evaluation will be performed by way of engine testing in a **Cummins 6.7L medium duty MCCI engine** at the CSU Powerhouse.
- High speed combustion, fuel consumption, and emissions (PM mass/number, 5-gas, and HC speciation) data

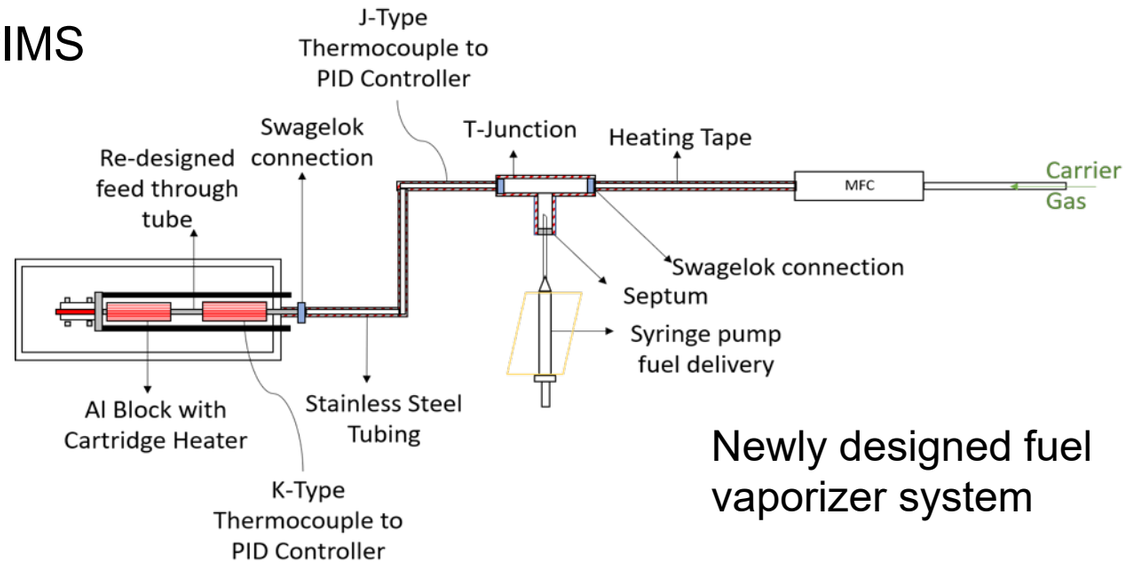
4- Progress and Outcomes - Kinetics

Subtask 2.1: Fundamental Chemistry Experiments Using μR-PIMS

Experimental Purpose: Microreactor experiments using photoionization mass spectrometry provide direct evidence of the likely dominant reaction products of POMEs under pyrolysis (no presence of O_2) conditions as a function of temperature. (see top fig. for setup)

Example Results: M-1-M pyrolysis experiments reveals pyrolysis products at m/z 15 for CH_3, indicating bond fission and rapid dissociation of the resultant radicals to methyl, formaldehyde (undetectable, IE = 10.88 eV) and H-atom (undetectable, IE = 13.60 eV).

Implications of Results: Both chain length and POME end groups directly impact the dilution effect (number of formaldehydes formed), reaction product distribution (production of species beyond CH_2O, CH_3, and H), and the onset temperature of observed chemistry (relative rate of reaction). These experiments can directly probe these chemical behavior differences and help identify ideal POMEs for production.



Newly designed fuel vaporizer system