Goals, Expected Outcomes, and Relevance

- **Goal:** Determine the technical feasibility of using biofuels, especially bio-oils for marine engine use
  - Feasibility determined by compatibility, emissions reduction, & efficiency improvement

- **Expected Outcome:** Understand the efficacy of biofuels in marine transport
  - Determine impact on fuel handling systems
  - Determine impact of bio-oils blended with market heavy fuel oils (HFO)
  - Identify technical needs associated with bio-oil use as fuel

- **Relevance:** Bio-oil and biocrude offer potentially viable fuels for marine engines currently powered using low-quality HFO
  - Pathway towards reduction of sulfur and particulate emissions
  - Reduced CO$_2$ emissions (lower carbon fuels)
  - Potential path towards improved efficiency (further CO$_2$ reduction)
  - Identify new market opportunities for bioenergy and bioproducts
Background: Marine Shipping Market

- Over 90% of all goods are shipped via marine vessels fueled with heavy residual fuel oil (HFO)
  - 40,000 ships worldwide burn ~5.2 million barrels of fuel/day \(^1\) (higher than US aviation and on-road diesel combined)
  - Largest source of global anthropogenic sulfur emissions worldwide, and of black carbon in the Arctic
  - Important contributor to worldwide CO\(_2\) emissions (~2%)

- HFO requires significant on-board processing
  - Significant water and solid content must be removed
  - HFO is also highly viscous and must be heated to temperatures exceeding 90°C to achieve proper flow characteristics

- On-board processing requires:
  - Heaters: maintain flow
  - Separator: remove water & sludge
  - Holding tanks
  - Filters

- In spite of the added hardware & energy costs, HFO is most economical fuel

---

New emissions regulations from International Maritime Organization (IMO) create significant challenges.

Fuel sulfur cap: Reduced from 3.5% to 0.5% globally in 2020

“Very low sulfur fuel oil” (VLSFO)

Greenhouse Gas (GHG) emissions:
- Energy Efficient Design Index (EEDI) - present
- IMO mandate of 50% GHG reduction by 2050 (will require new low-carbon fuels)

Current lower-C fuels:
- LNG
- Biodiesel trials

Future net-zero C fuels:
- e-fuels
- Biofuels

LNG requires cryogenic storage and dramatically lowers cargo carrying capacity
Biofuels: Creative Advantage

Biofuels are an attractive option since they are inherently low in sulfur and provide lifecycle greenhouse gas benefits.

- Marine engines are designed to burn low-grade residuum and can operate effectively on low-combustion quality fuels.
- Bio-oils and biocrudes are expensive to upgrade to be miscible with distillates (diesel, etc.), but have drop-in potential with HFO.
- Compliance will raise operating costs such that biofuels may offer an economic alternative.
- In addition to reduced sulfur emissions, biofuels have much lower viscosity, which, if blended with HFO, would be expected to lower heating costs thereby increasing overall system efficiency.
Strong collaborations for stakeholder input and economic assessment

- Partners include DOE, DOT/MARAD (funds-in), and colleagues at NREL, PNNL, & ANL
- Work coordinated with larger multi-lab project evaluating potential impact of a marine bio-fuels program
- Regular communication through bi-weekly calls
- Bio-oils provided by colleagues at NREL & industry
- Collaboration with ExxonMobil SPP project to obtain 2-stroke research engine data

Team members and roles

- Mike Kass¹ (PI) – Project oversight, material & blend compatibility evaluation
- Brian Kaul¹ – Engine & combustion evaluation
- Flavio Chuahy² – Simulations & combustion modeling

¹Engine Technologies Research Group
²Combustion & Fuel Science Research Group

Project risks

- Blend instability/corrosivity
- Limited quantities of bio-fuels for evaluation
- Feasibility of collecting engine data
- Lack of good chemical kinetic mechanisms for engine simulations

Communication of results

- Technical publications
- Conference presentations
- Industry workshops
- Telecons and site visits to interested parties
Use experiments and analysis to fill gaps in understanding of bio-oil impacts/potential

• Understanding bio-oil properties & compatibility with current market fuel (VLSFO)
  – ASTM D4740 Miscibility (solubility) determination to ensure that asphaltenes are not precipitated from the VLSFO
  – Viscosity measurement in the relevant temperature ranges to ensure fuel system handling of bio-oil/VLSFO blends
  – Corrosion testing to ensure material compatibility
  – Combustion testing to confirm engine suitability
Use experiments and analysis to fill gaps in understanding of bio-oil impacts/potential

- Understanding bio-oil properties & compatibility with current market fuel (VLSFO)
  - ASTM D4740 Miscibility (solubility) determination to ensure that asphaltenes are not precipitated from the VLSFO
  - Viscosity measurement in the relevant temperature ranges to ensure fuel system handling of bio-oil/VLSFO blends
  - Corrosion testing to ensure material compatibility
  - Combustion testing to confirm engine suitability

- Understanding bio-oil impact on engine performance

Two distinct technologies: 4- and 2-stroke engines have substantially different fuel requirements
Use experiments and analysis to fill gaps in understanding of bio-oil impacts/potential

- Understanding bio-oil properties & compatibility with current market fuel (VLSFO)
  - ASTM D4740 Miscibility (solubility) determination to ensure that asphaltenes are not precipitated from the VLSFO
  - Viscosity measurement in the relevant temperature ranges to ensure fuel system handling of bio-oil/VLSFO blends
  - Corrosion testing to ensure material compatibility
  - Combustion testing to confirm engine suitability

- Understanding bio-oil impact on engine performance
  - Computational evaluation of performance of candidate bio-fuels using digital twin of 2-stroke crosshead research engine
    - Verify CFD model using diesel/VLSFO data from ExxonMobil “Enterprise” 1:10 scale single-cylinder research engine at ORNL
    - Evaluate performance of candidate fuels using known properties
      - Bio-diesel, bio-oils; baseline vs. VLSFO/diesel and other future fuels, e.g. ammonia, alcohols
      - Determine technical and economic feasibility of establishing capability for obtaining 4-stroke-relevant data
Challenges and Measures of Success

• Potential challenges
  – Lack of available information
  – Excessive bio-oil polymerization
  – Lack of suitable quantities of biofuels for evaluation
  – Removal of retained water
  – Difficulty of obtaining relevant engine performance data

• Critical success factors (technical, market, business)
  – Reduced blend viscosities
  – Efficient combustion with lowered PM formation
  – Compatibility with existing infrastructure

• A go/No-go decision was met during FY19 concerning the possibility of polymerization of the bio-oil in blends containing HFO at elevated temperatures. Since this was determined to not be an issue, the decision was made to go forward with the project as planned.
Marine emissions among hardest to eliminate: potential for significant near-term impact

Shipping emissions account for 18% of global transportation-sourced 20-year CO₂-equivalent global warming potential

IMO Mandate: 50% GHG reduction by 2050: Only possible with new low-carbon and net-zero carbon fuels & engines

Large potential market for biomass and biofuels: global shipping consumes 300 Mt/year

Modeling study will be of enormous benefit to industry: provides a means of assessing performance, saving time and expense associated with expensive engine screening

“Smith et al. (2015) estimate that ship CO₂ emissions will increase 50%–250% from 2012 to 2050, and CE Delft (2017) projects that emissions will increase 20%–120% over the same period for global temperature rise scenarios less than 2°C”
Marine emissions among hardest to eliminate: potential for significant near-term impact

Shipping emissions account for 18% of global transportation-sourced 20-year CO₂-equivalent global warming potential.

IMO Mandate: 50% GHG reduction by 2050: Only possible with new low-carbon and net-zero carbon fuels & engines.

Large potential market for biomass and biofuels: global shipping consumes 300 Mt/year.

Modeling study will be of enormous benefit to industry: provides a means of assessing performance, saving time and expense associated with expensive engine screening.

Findings disseminated to the shipping industry as part of a BETO sponsored workshop at the CMA Shipping 2020 Conference.

Results presented and disseminated to stakeholders including:

- Maersk Oil and Gas Climate Initiative
- MAN EPA and DOT
- ExxonMobil World Shipping Council
- GoodFuels Biofuels Digest
- Blue Insight DNV-GL
- Ensyn Crowley

Compatibility/stability and corrosion results favorable for bio-oil use

- Bio-oil can be blended with VLSFO without significant asphaltene precipitation
  - Blend stability testing conducted using ASTM D4740
  - Polymerization of the bio-oil was impeded by blending
- Negligible corrosion for blends up to 50% bio-oil

### Corrosion rates of various steels at 50°C

<table>
<thead>
<tr>
<th>Bio-oil content (mass%)</th>
<th>Carbon Steel</th>
<th>2.25Cr– 1Mo Steel</th>
<th>409 Stainless Steel</th>
<th>304L Stainless Steel</th>
<th>316L Stainless Steel</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>250h</td>
<td>500h</td>
<td>250h</td>
<td>500h</td>
<td>250h</td>
</tr>
<tr>
<td>8</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>19</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>25</td>
<td>0.02</td>
<td>0.03</td>
<td>&lt;0.01</td>
<td>0.07</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>50</td>
<td>0.05</td>
<td>0.04</td>
<td>0.09</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>100</td>
<td>1.97</td>
<td>1.69</td>
<td>4.82</td>
<td>2.83</td>
<td>1.32</td>
</tr>
</tbody>
</table>
Combustion properties favorable for up to 15% bio-oil blends, with significant viscosity benefit

- Viscosity of VLSFO was dramatically lowered by small additions of bio-oil
- Combustion analysis showed that blends containing up to 15% bio-oil were acceptable as drop-in replacements
  - Tests were conducted by an independent laboratory, and estimated cetane numbers were all in suitable range
  - Higher blends could not be tested in fuel combustion analyzer due to polymerization at standard high-temperature conditions
  - Higher blends may be feasible with changes to engine/process controls due to reduced heating requirements

Viscosity of VLSFO was dramatically lowered when 5% bio-oil was added

**Progress and Outcomes**

- Reduced viscosity
  ⇒  Reduced fuel heating energy requirement
Established capability for evaluating bio-oil impacts in marine engines

• Established digital twin of “Enterprise” 2-stroke research engine
  – Verified digital twin model performance against existing data w/ diesel fuel
  – Developed reduced kinetics models & surrogate fuels for biodiesel & bio-oil based on available literature
  – Simulations being conducted on internal “CADES” cluster and with an awarded allocation on NREL “Eagle” high performance cluster

• Evaluating options for 4-stroke engine experimental platform
  – Potentially leverage HFO treatment/handling capabilities from ExxonMobil strategic partnerships project
  – Provide data on 4-stroke engine combustion impacts
  – Provide validation data to enable simulations/digital twin studies as with 2-stroke engines
  – Scoping study currently in progress
Developed reduced chemical kinetic mechanism for simulating bio-oil combustion

- Reaction chemical mechanisms developed for:
  - Biodiesel, Bio-oil, and ultra-low-sulfur diesel (ULSD) fuels
  - Estimation of NO$_x$ and soot precursor (polycyclic aromatic hydrocarbons (PAH)) formation

- Detailed mechanism from CRECK group used as base
  - Reduced mechanisms developed for each fuel of interest using a direct relation graph with error propagation (DRGEP) method
  - Sub mechanism developed for PAH chemistry up to Pyrene to represent soot formation potential

- Mechanism retains large number of species for accurate predictions

Developed mechanisms allow the study of NO$_x$ and soot precursor (PAH) formation for different bio-derived fuels.
Good simulation performance ⇒ established digital twin capability for screening bio-fuels

- Excellent agreement between model and experimental data with ULSD fuel
  - Grid independence study conducted to find optimal grid resolution
  - Heat release rate was very well captured by the model
    - Transition of first-injection ignition to second-injection ignition is captured accurately
  - \(\text{NO}_x\) emissions match experimental values

<table>
<thead>
<tr>
<th>NO(_x) Emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiments</td>
</tr>
<tr>
<td>Simulations</td>
</tr>
</tbody>
</table>

Digital twin simulations will be used to screen bio-fuel candidates for 2-stroke marine engine combustion and emissions

Future work will study sources of PAH and NO\(_x\) emissions and compare against bio-diesel and bio-oil mixtures
Initial bio-oil compatibility looks promising; further study will elucidate engine impacts

- Initial studies show that bio-oils:
  - Are suitable for blends with VLSFO: good compatibility and stability
  - Reduce the viscosity of VLSFO: potential increase in efficiency via reduced fuel heating
  - Are not corrosive to fuel system metals at blends up to 50%
  - Show acceptable combustion properties for blends up to at least 15%

- Digital twin simulation capability established for 2-stroke crosshead engine
  - Digital twin model was developed and verified against experiments
  - Excellent agreement in NO\textsubscript{x} emissions between digital twin and experiments
  - Reduced reaction mechanisms were developed for fuels of interest ⇒ Enable analysis of bio-
    diesel and bio-oil blends against baseline simulations
  - Mechanisms incorporate soot precursor chemistry to estimate soot formation
  - Digital twin is now capable of exploring bio-fuel efficiency and emissions trade-offs

- Options for obtaining 4-stroke-relevant engine data are being scoped out
### Timeline
- **Project start date:** Oct 1, 2017
- **Project end date:** March 31, 2021 (currently)

<table>
<thead>
<tr>
<th>DOE Funding</th>
<th>FY21</th>
<th>Active Project</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$495k</td>
<td>FY21</td>
</tr>
<tr>
<td></td>
<td>$1,100k (total)</td>
<td>FY18-FY21</td>
</tr>
</tbody>
</table>

### Project Goal
This effort seeks to determine the feasibility of biofuels (especially bio-intermediates) as viable fuel candidates for marine engines.

### End of Project Milestone
Evaluate and quantify the opportunity of biofuel use in HFO-fueled marine engines in terms of efficiency and emissions potential.

### Project Partners
- **NREL** – supply bio-oils
- **ExxonMobil** – engine data
- **Ensyn** – provide bio-oils for compatibility assessments

### Barriers addressed
- **Pm-A. Strategy and Goals**
- **At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts**

### Funding Mechanism
AOP
Additional Slides
Responses to Previous Reviewers’ Comments

- Report was viewed favorably
- Need to engage stakeholders was accomplished through web meetings and workshop at CMA Shipping 2020 Conference
Publications, Patents, Presentations, Awards, and Commercialization