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NNSA Laboratory Directed Research & Development

Energy Use Impacts and Mitigation

Tailoring Next-Generation Biofuels and their Combustion in Next-Generation Engines

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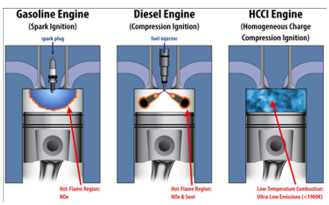
What is the challenge?

The global need for energy is subject to increasing carbon constraints because of the challenges of climate change. Moreover, for energy security it is desirable to have reliable domestic fuel supplies.

Biofuels are a potential domestic source of transportation fuels with a reduced carbon footprint, addressing energy security, economic competitiveness, and global climate concerns. However, current biofuels offer only relatively small reduction in greenhouse gas emissions, and limited economic viability. As a result, new methods are being sought that will convert lignocellulosic biomass into useful transportation fuels. This quest is extremely challenging because of the difficultly and expense of breaking down lignin and cellulose.

Effective deployment of biofuels may entail a substantial change in fuel chemistry

Operation of spark-ignition, diesel, and advanced compression-ignition engines. Emerging engine designs, of which HCCI is one example, promise increased efficiency and reduced pollutant emission,



At the same time that fuels are changing, new designs for clean, efficient combustion engines are increasingly sensitive to the details of fuel chemistry.

New combustion strategies that use compression ignition of a lean and dilute mixture can deliver high efficiency while maintaining low combustion temperatures that prevent formation of nitrogen oxide pollutants. However, the combustion timing depends on fuel autoignition chemistry. The control strategies required to operate such engines reliably over a full range of loads and speeds may change with changing fuels.

Coordination of fuel and engine development could help *enable* new engine technologies

What is our innovation?

Development of a robust framework for linking biofuel production to investigations of combustion performance

- In the initial design of a new biomass conversion platform, potential biofuels are identified
- Biofuels whose combustion behavior is not already well characterized are subjected to fundamental combustion studies and models for engine performance are developed
- The optimization of the biofuel production is steered towards compounds with advantageous combustion chemistry
- Adaptable framework – beyond any specific set of platforms, represents a new way to engineer biofuels

This framework is demonstrated and exploited in the development of new biofuel platforms based on the metabolic pathways of endophytic fungi

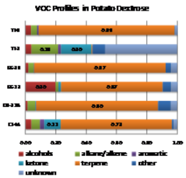
- Fungal endophytes live in a symbiotic relationship with a host woody plant and naturally consume lignocellulosic biomass to produce useful volatile organic compounds (VOCs) with high energy density and great potential as diesel or fuel additive replacements.
- Endophytic fungi produce a wide spectrum of cellulosic and lignin degradation enzymes
- Synthetic biology tools can discover and exploit the metabolic pathways of these fungi to develop a potential consolidated bioprocessing method, avoiding expensive pretreatment

Endophytic fungus *Hypoxylon* sp. CO27 after nine days of growth on minimally processed switchgrass

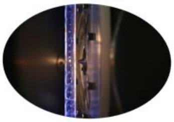
What have we learned so far?

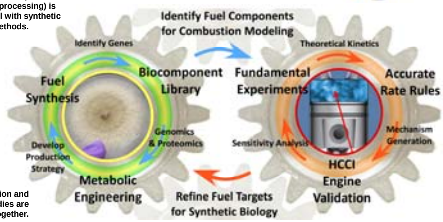
Natural products of the endophytes include ketones, whose ignition chemistry is poorly known.

Direct VOC production from fungal action on biomass (i.e., consolidated bioprocessing) is pursued in parallel with synthetic biology methods.

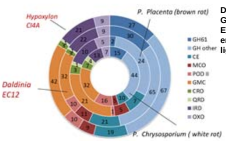


Laser-initiated experiments probe the chemical kinetics of key elementary ketone combustion reactions, helping to develop chemical mechanisms .



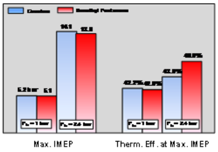


Biofuel production and utilization studies are meshed together.



Distribution of Oxidative Lignin Genes in Endophyte Genomes. Endophytes have machinery for enzymatic and non-enzymatic lignocellulose degradation.

Some ketones show improved efficiency in HCCI engines over gasoline at similar load (IMEP). New chemical mechanisms successfully predict engine pressure profiles.



Four strains of endophytic fungi have been investigated and their metabolic pathways analyzed

- All strains show abundant and powerful enzymes for degrading lignocellulosic biomass
- Endophytes expressed different cellulase activities on different feedstocks.
- Pathways for synthesis of biofuel compounds and breakdown of lignocellulose can be expressed in tractable organisms for process scale-up

Ketone fuels identified as potentially useful products of fungal metabolism

- Ketone chemistry previously poorly characterized, but fundamental experiments and calculations developed new combustion mechanism
- HCCI engine investigations showed high efficiency at high load for ketone fuel

Why is this important for our nation?

Co-engineering of biofuel production and combustion increases the impact of both processes

- Utilization of new biofuels will be facilitated by combustion models that can predict their performance in existing and future engines
- Control of biofuel combustion properties can ensure that higher efficiency and cleaner combustion engines are not hindered, and may be enhanced, by new fuel chemistry
- Improvements in combustion efficiency, increased domestic sourcing of transportation fuels, and national technological expertise in low-net-carbon energy are likely to be critical economic advantages for the U.S.

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