

# High Pressure Ignition Chemistry of Alternative Fuels

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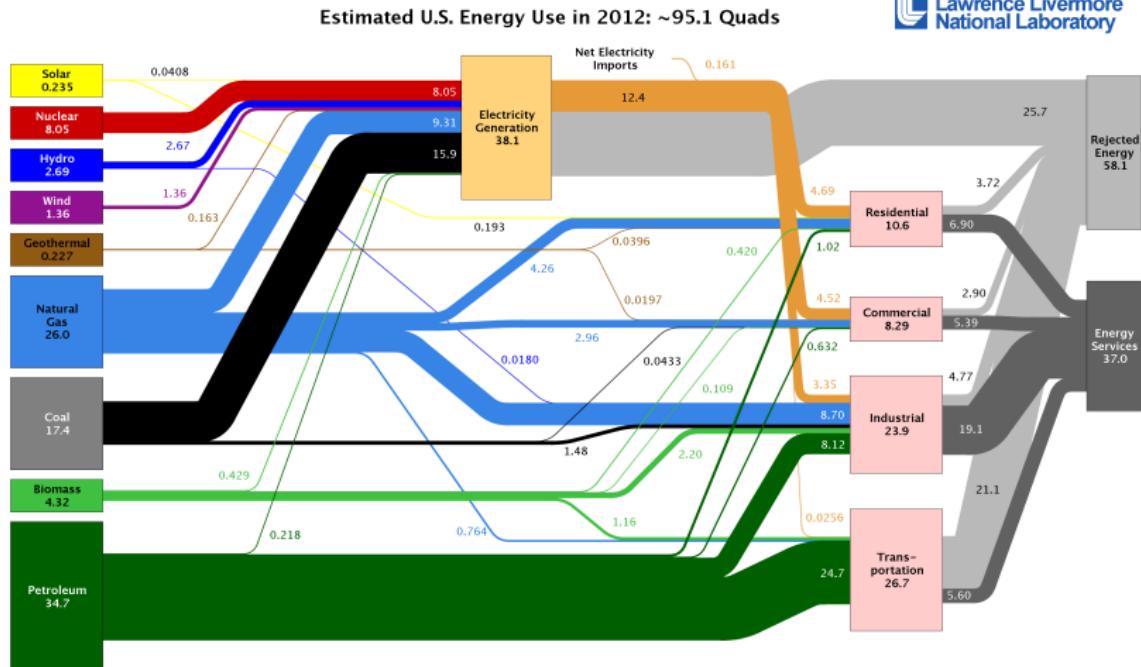


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# We use a lot of fuels to power the world

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# We use a lot of fuels to power the world

Could drive to the moon and back over 150 million times in a Tesla with the amount of energy we use annually

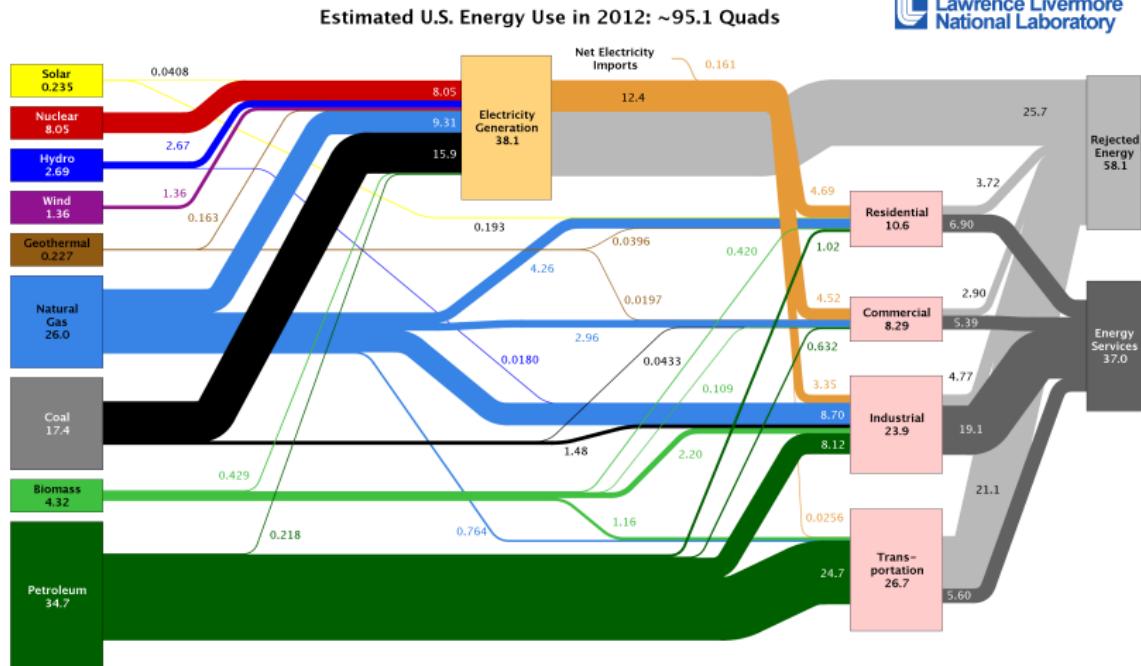


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# We use a lot of fuels to power the world

- ▶ Combustion is predicted to remain the dominant energy conversion process for many years into the future
- ▶ The combustion of fossil fuels has been implicated in a number of harmful effects on human health, the environment, and the economy
- ▶ Two solutions have been proposed:
  - ▶ Better engines
  - ▶ Better fuels

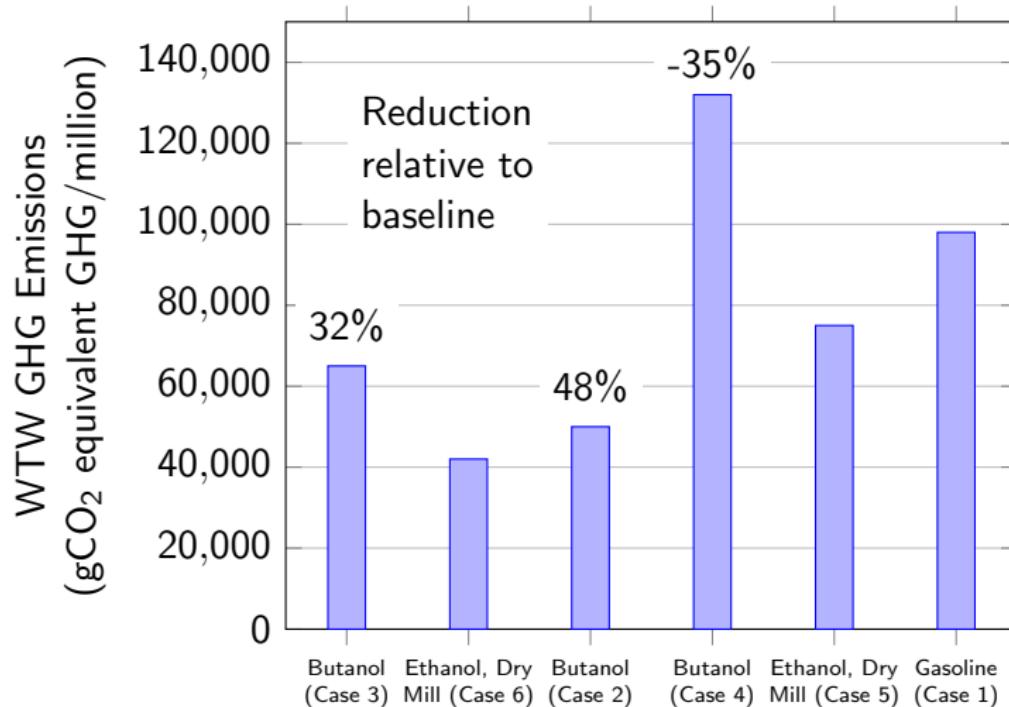


# Better engines have higher efficiency and lower emissions

John Dec image



# Better fuels reduce emissions and eliminate dependence on fossil fuels



## We need both solutions to make substantial progress

- ▶ Neither solution will be able to mitigate all of the negative impacts of combustion by itself
- ▶ Selecting the best alternative fuel requires knowledge of the best engine, which depends on which alternative fuel is selected
- ▶ Computer-aided design and modeling can be employed to make new engines fuel-flexible **if we have good models**
- ▶ Models must be validated with experimental data acquired under engine-relevant conditions



# Combustion models are hierarchical

- ▶ In this, “combustion models” = “kinetic models” = “reaction mechanisms”
- ▶ Combustion chemistry is important!  
Studied since at least the advent of IC engines to understand knock; later for emissions and pollutants.
- ▶ Need to ensure that the models for small molecules are thoroughly validated when including them in models for large molecules
- ▶ A number of research efforts (past and present) have focused on this goal

H<sub>2</sub>, CO



# Combustion models are hierarchical

- ▶ Model validation for larger molecule combustion must proceed in parallel to the small molecule chemistry because the models are needed now!
- ▶ Validation data for alcoholic alternative fuels has focused on the isomers of butanol (C4 alcohols) and i-pentanol (C5 alcohol)



## Combustion models are hierarchical

- ▶ Models can predict the combustion of alcohols well for a variety conditions
- ▶ Models fail to predict certain engine relevant conditions, such as ignition delay dependence on  $[O_2]$



## Combustion models are hierarchical

- ▶ Models of real transportation fuels are difficult to construct and use due to the chemical complexity of the fuels
- ▶ Surrogate models use a limited number of components to represent the chemical and physical properties of the real fuel
- ▶ Models need to be developed and validated for the neat components as well as for their blends



# Summary

- ▶ We need a better understanding of the combustion properties of fuels we use now, fuels for the medium-term, and fuels for the long-term especially under engine-relevant conditions
- ▶ Using this understanding, we need to develop models that can predict the combustion behavior of new fuels in new engines
- ▶ My dissertation did x y z to advance these causes



# Why Bio-Alcohols?



# Why MCH?

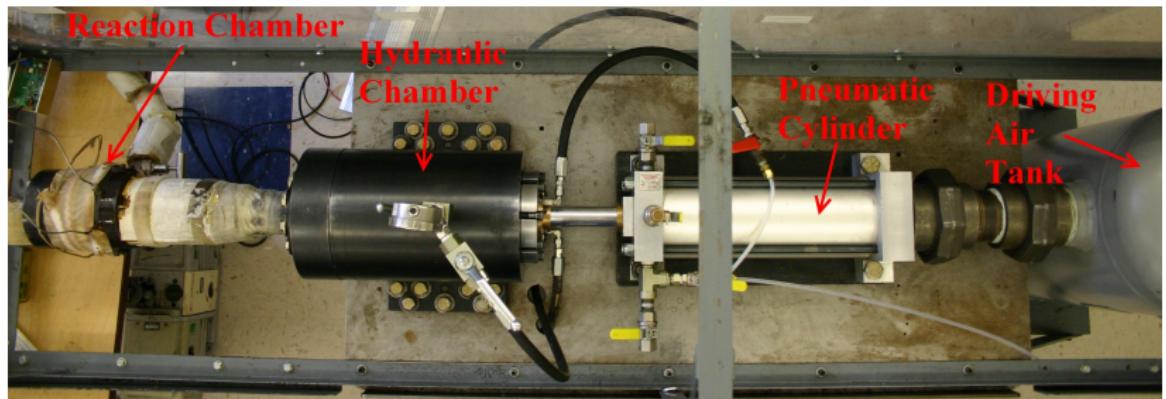
What are surrogates? (Has been touched on briefly previously)



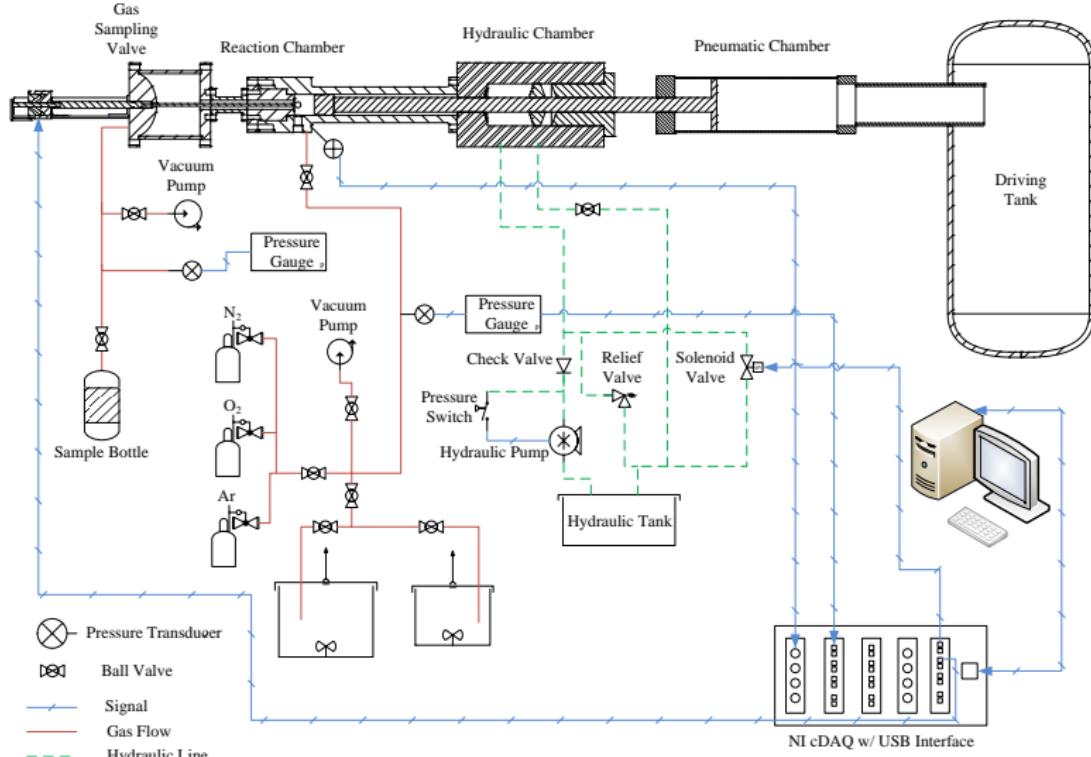
# Experimental Apparatuses



# Rapid Compression Machine



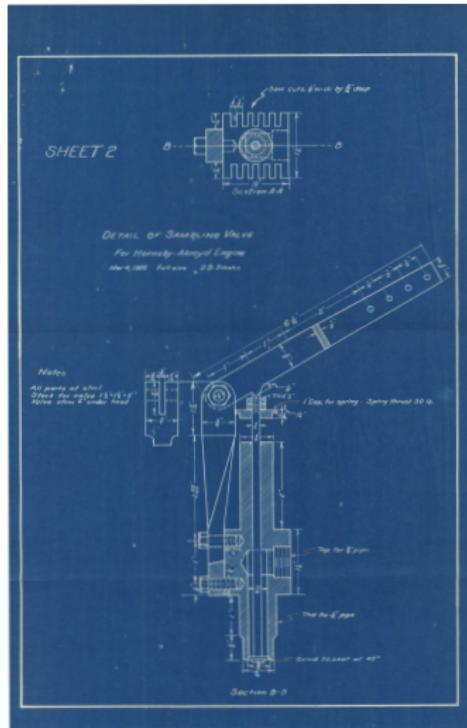
# Rapid Compression Machine



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# Rapid Sampling Apparatus

- ▶ Sampling apparatuses have been used since the 1920's to study combustion chemistry

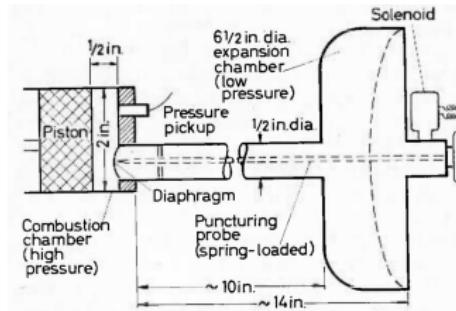


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- ▶ In the 1960's, the first sampling apparatus was adapted for an RCM
- ▶ Mittal developed a similar system for the present RCM based on deactivating an electromagnet
- ▶ I have modified the design of Mittal to incorporate a solenoid instead of the electromagnet



# Gas Chromatograph/Mass Spectrometer

- ▶ Standard piece of chemistry lab equipment, commercially supplied (Shimadzu)
- ▶ Separates, identifies, and quantifies chemical species

