

High Pressure Ignition Chemistry of Alternative Fuels

Bryan W. Weber

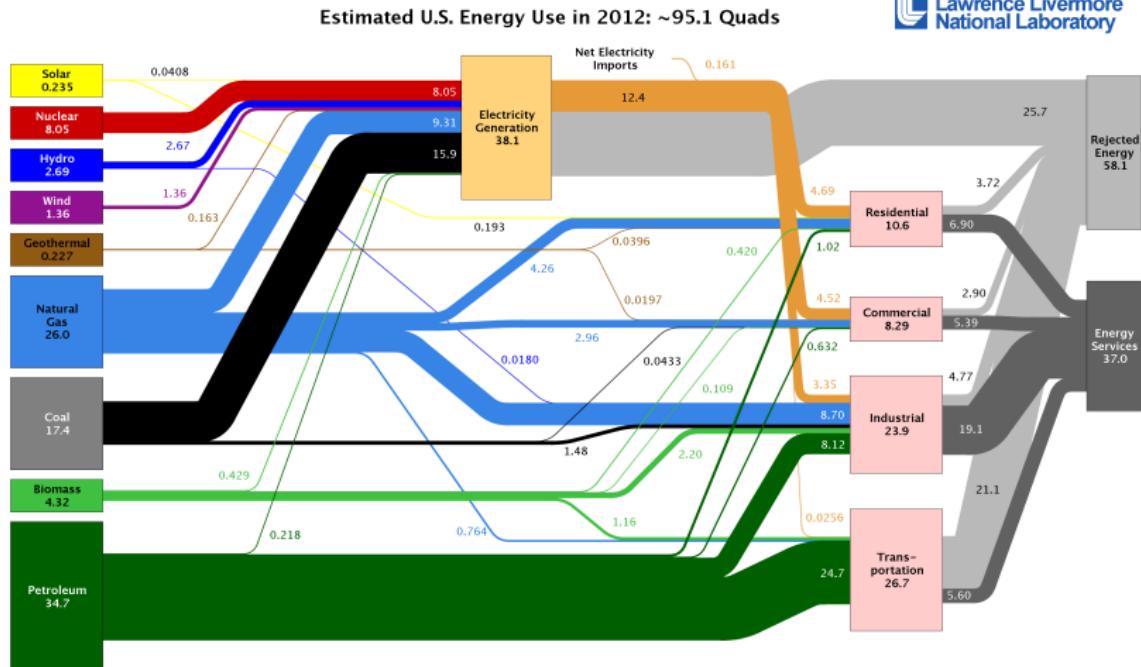
Prepared for Ph.D. Defense

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We use a lot of fuels to power the world

Lawrence Livermore National Laboratory



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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

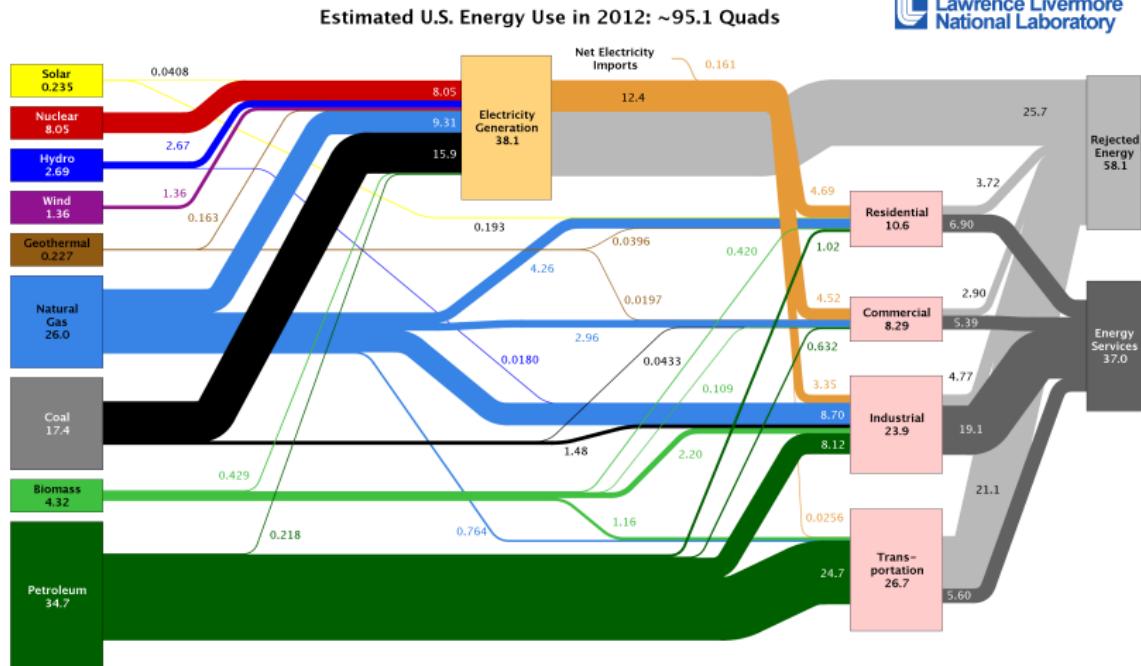


UCONN
COMBUSTION
DIAGNOSTICS
LABORATORY



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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

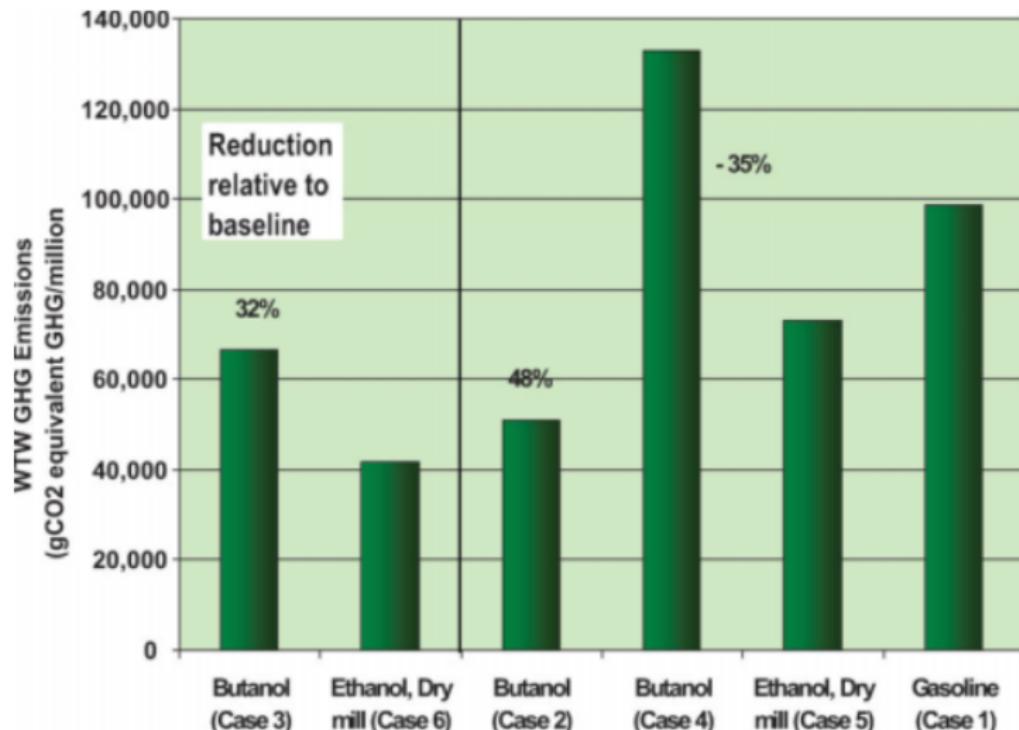


Better engines have higher efficiency and lower emissions

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

H₂, 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



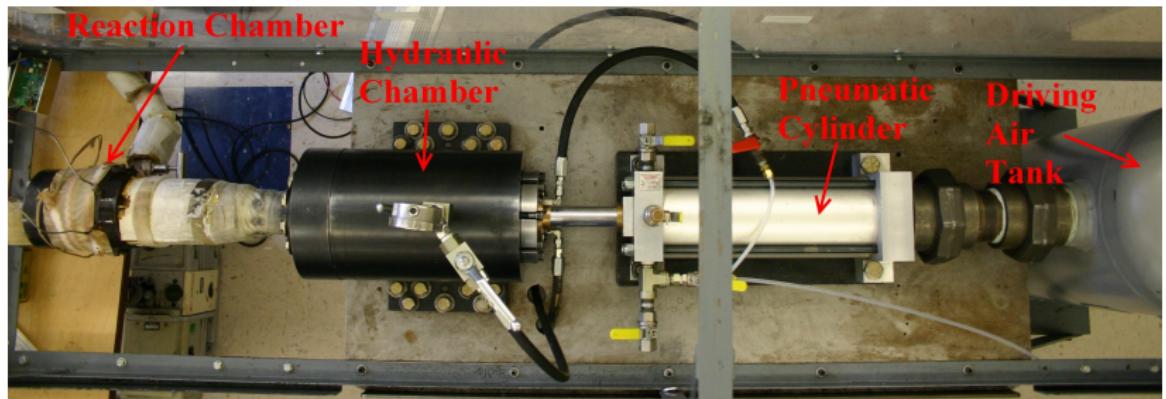
Why Butanol?



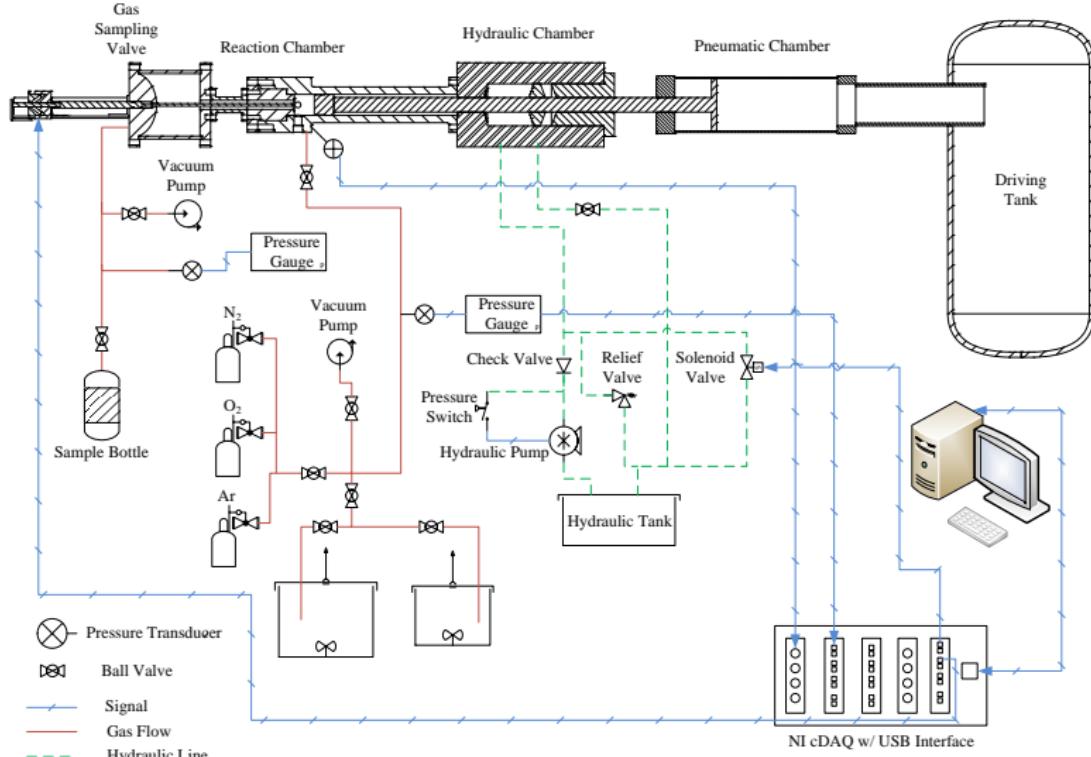
Experimental Apparatuses



Rapid Compression Machine

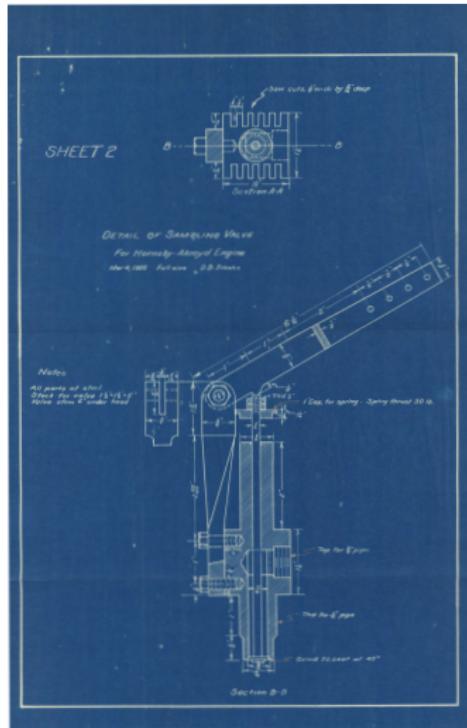


Rapid Compression Machine



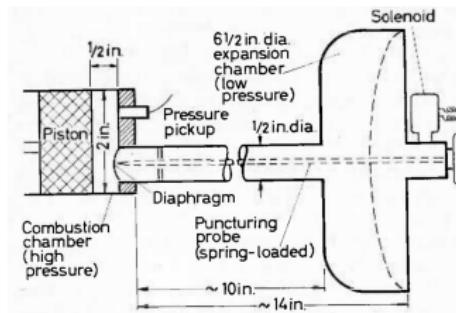
Rapid Sampling Apparatus

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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

