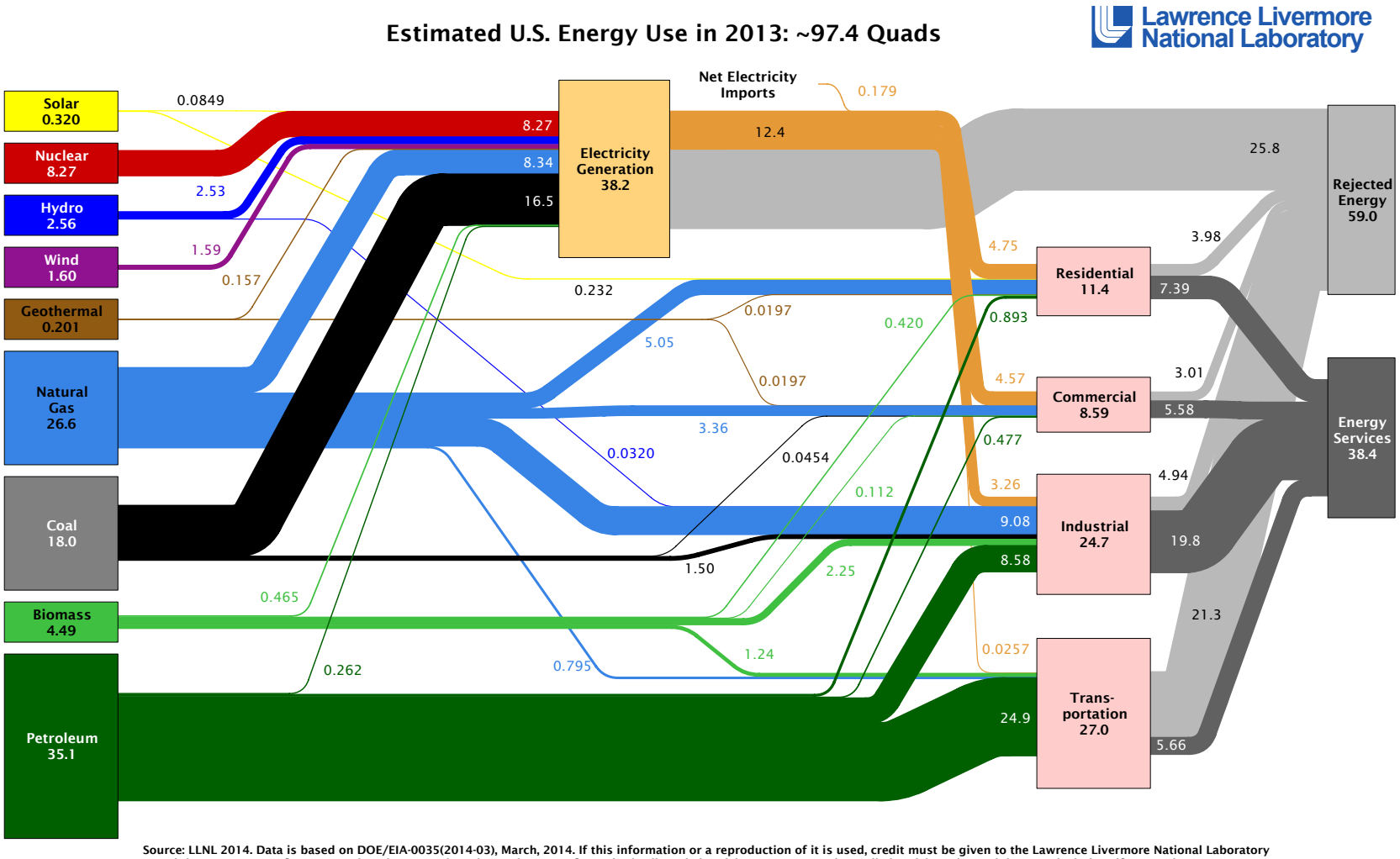
High Pressure Ignition Chemistry of Alternative Fuels

Bryan W. Weber

Prepared for Ph.D. Defense

June 19, 2014

We use a lot of fuels to power the world



Source: LLNL 2014. Data is based on DOE/EIA-0035(2014-03), March, 2014. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential and commercial sectors 80% for the industrial sector, and 21% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

We use a lot of fuels to power the world

Could drive to the moon and back over 180 million times in a Telsa Model S with the amount of energy we use annually

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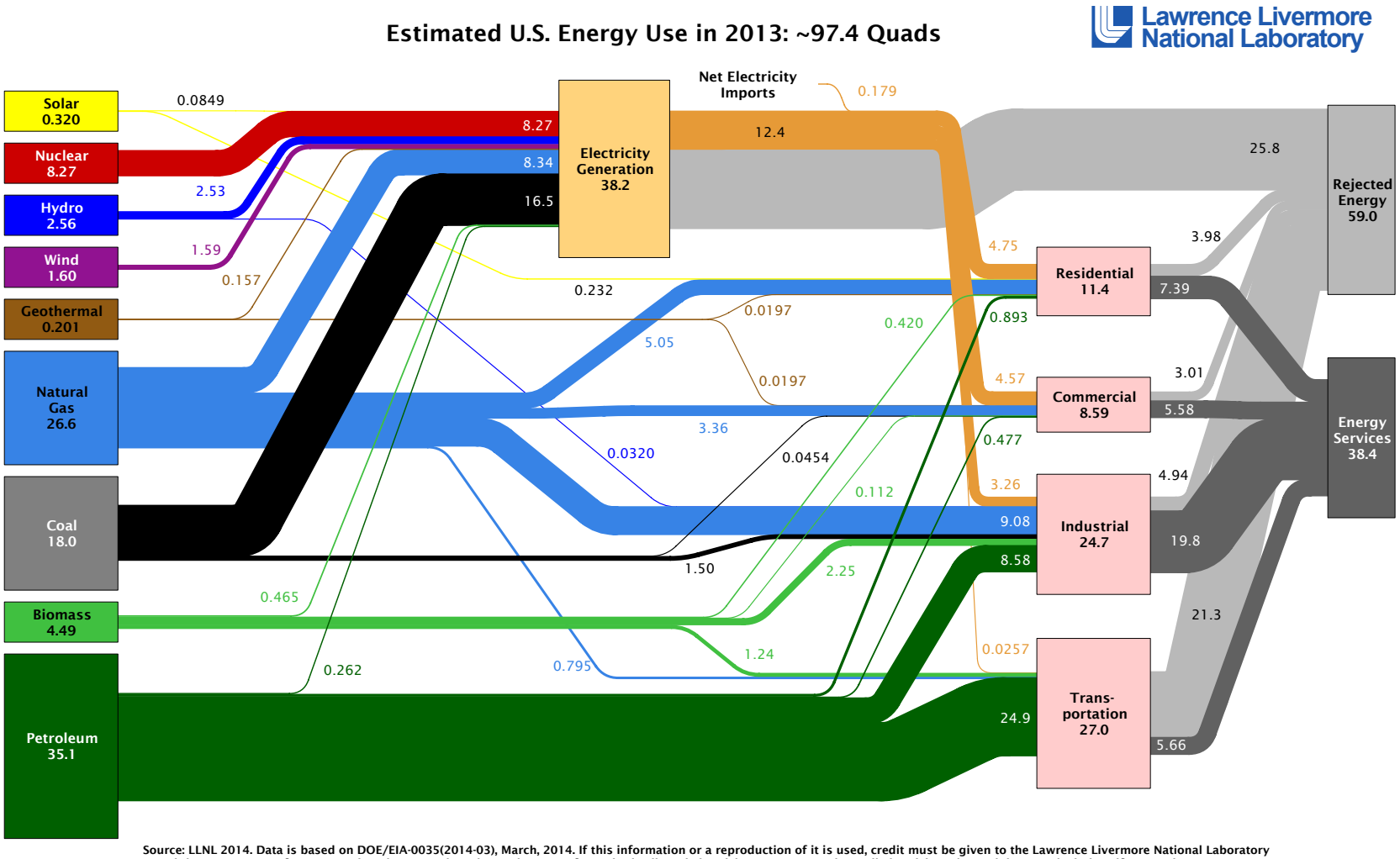

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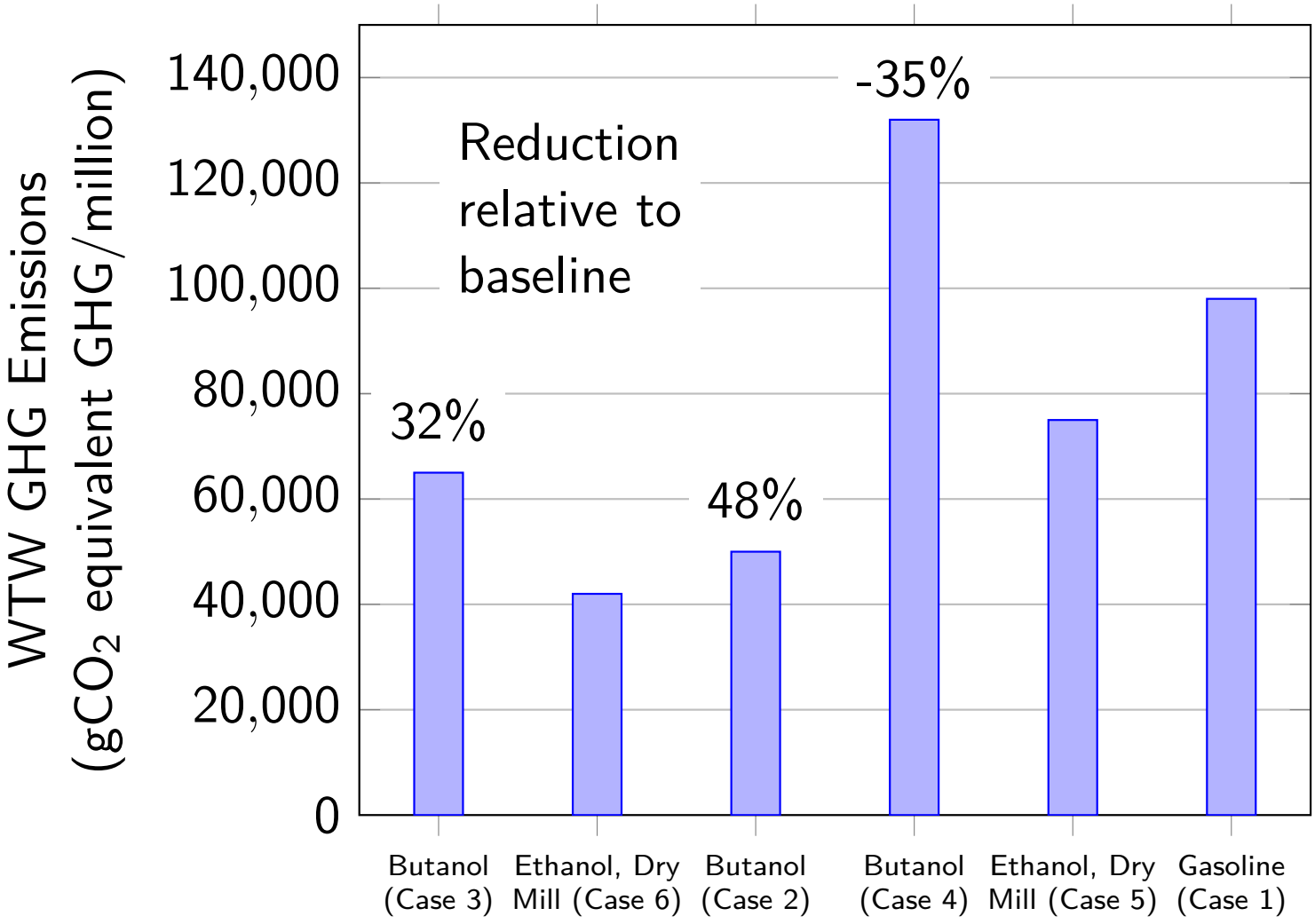
We use a lot of fuels to power the world

- 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

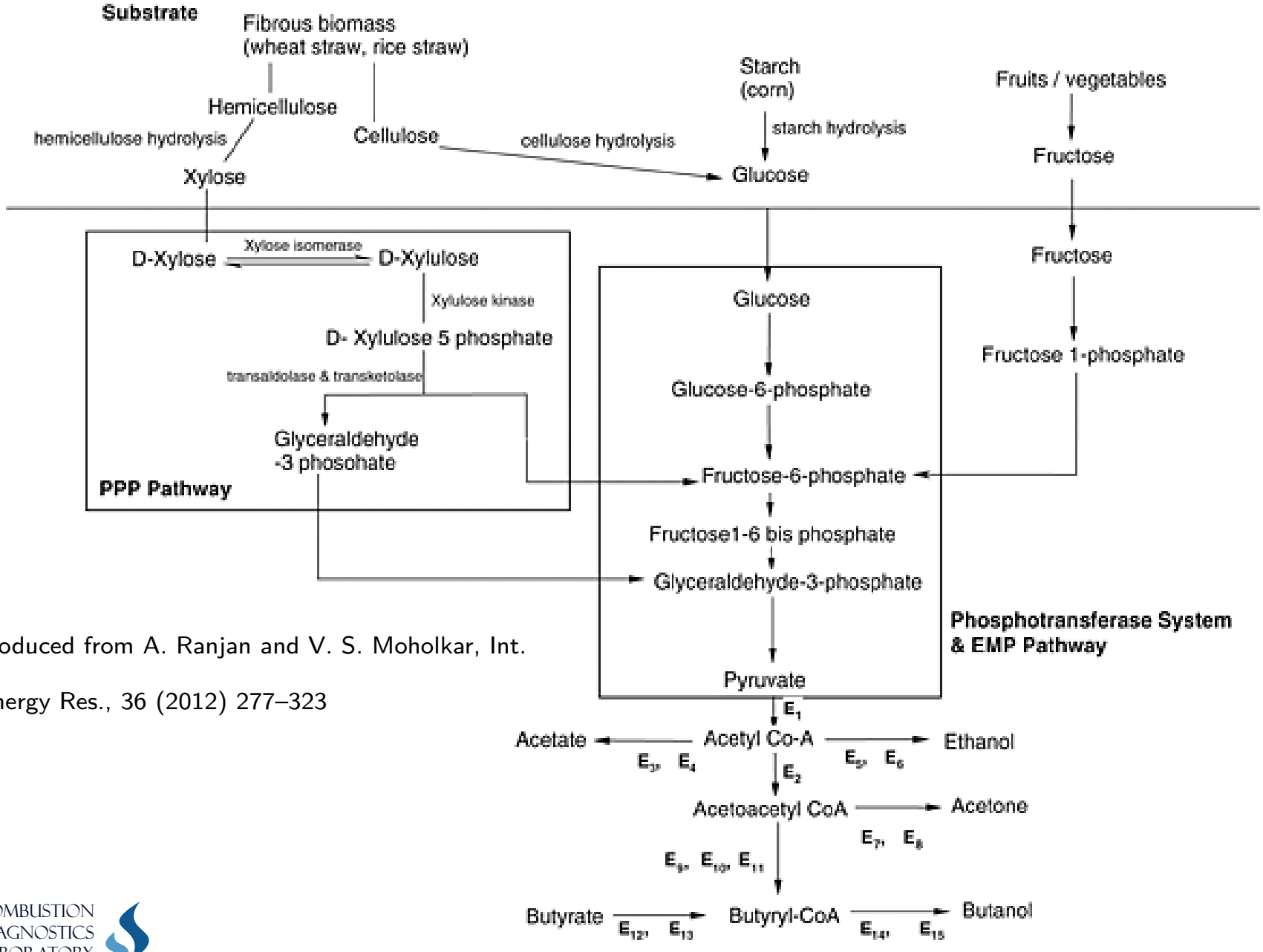
Better fuels reduce emissions and eliminate dependence on fossil fuels



Reproduced from M. Wu, M. Wang, J. Liu, H. Huo, Biotechnol. Prog. 24 (2008) 1204–1214.

What kind of research can we do to push these solutions along?

We can do biological research to produce the fuels



Reproduced from A. Ranjan and V. S. Moholkar, Int. J. Energy Res., 36 (2012) 277–323

We can do engineering research on how the fuels will behave

- We need to know the physical properties
  - Density
  - Viscosity
  - ...
- We need to know the combustion properties
  - Heat of combustion
  - Propensity to generate pollutants
  - Reactivity
  - ...

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What tools can combustion research use?

Phenomenological Studies

- Engine Studies
- Octane Number
- ...

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Fundamental Studies

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- Experiments

- Modeling

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  - Quantum chemical modeling
  - Reaction mechanisms
  - Computational fluid dynamics

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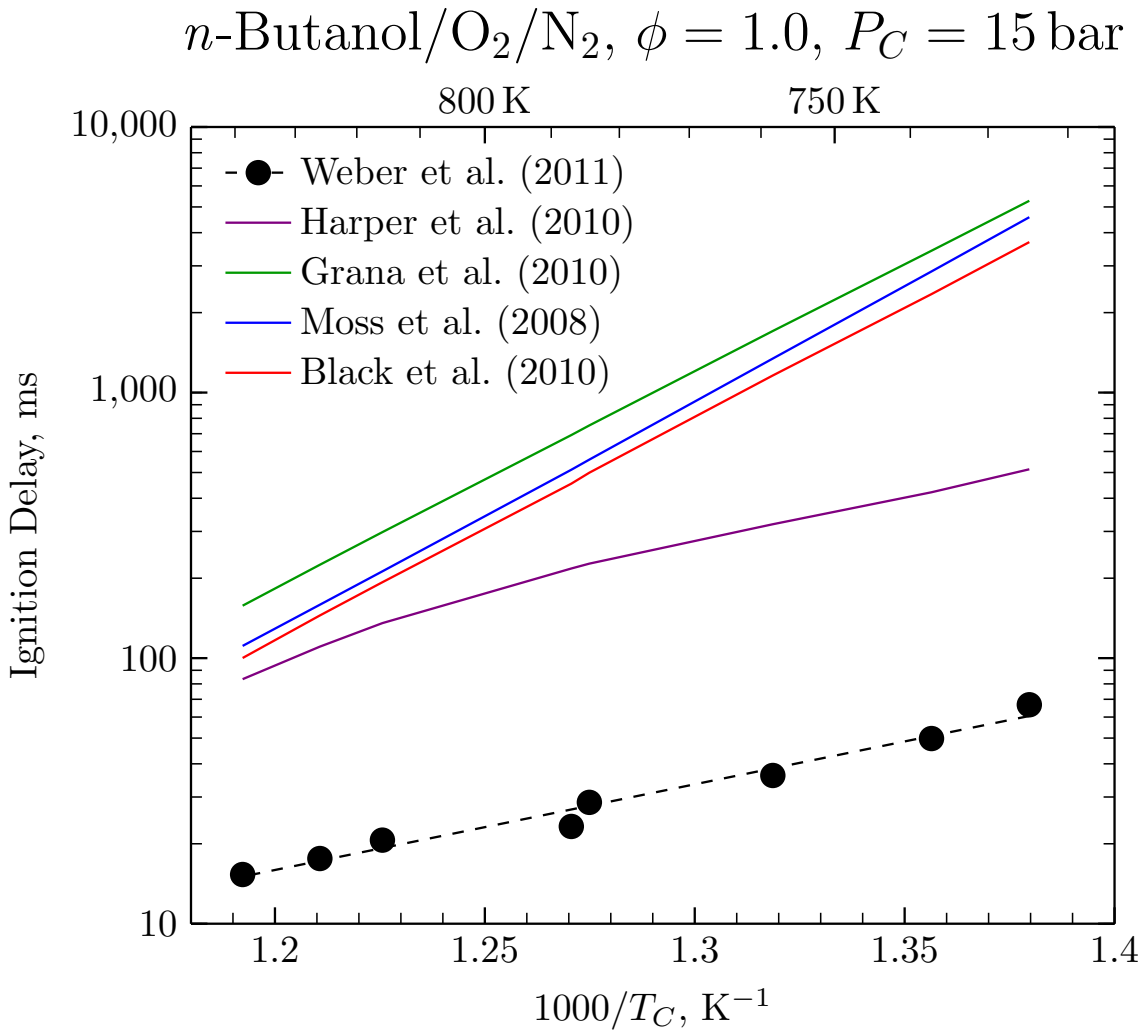
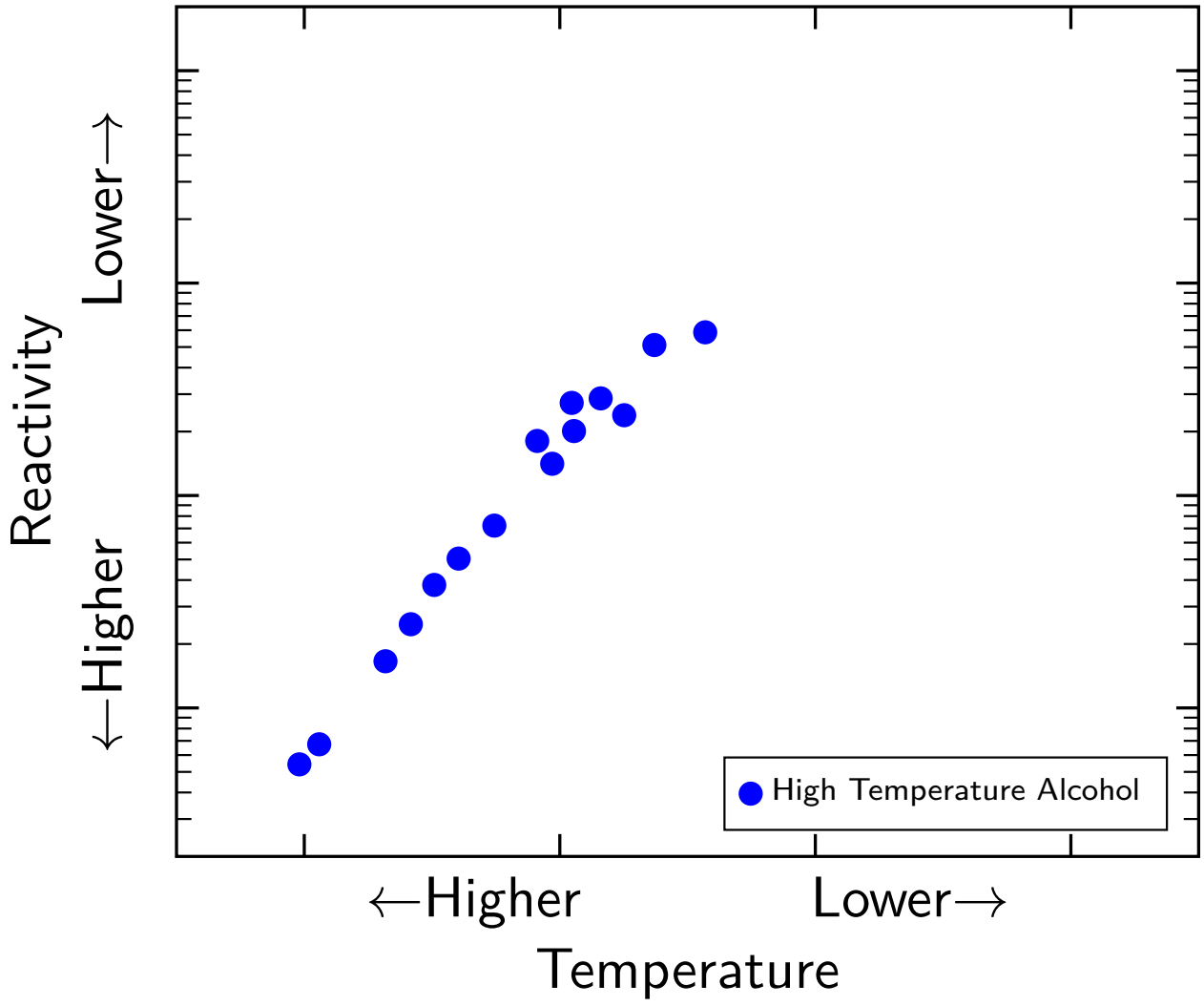
These efforts are complementary!

What problem am I trying to solve?



Until 2011, no one was aware that low-temperature chemistry would be important for alcohol fuels!

What is low-temperature chemistry?



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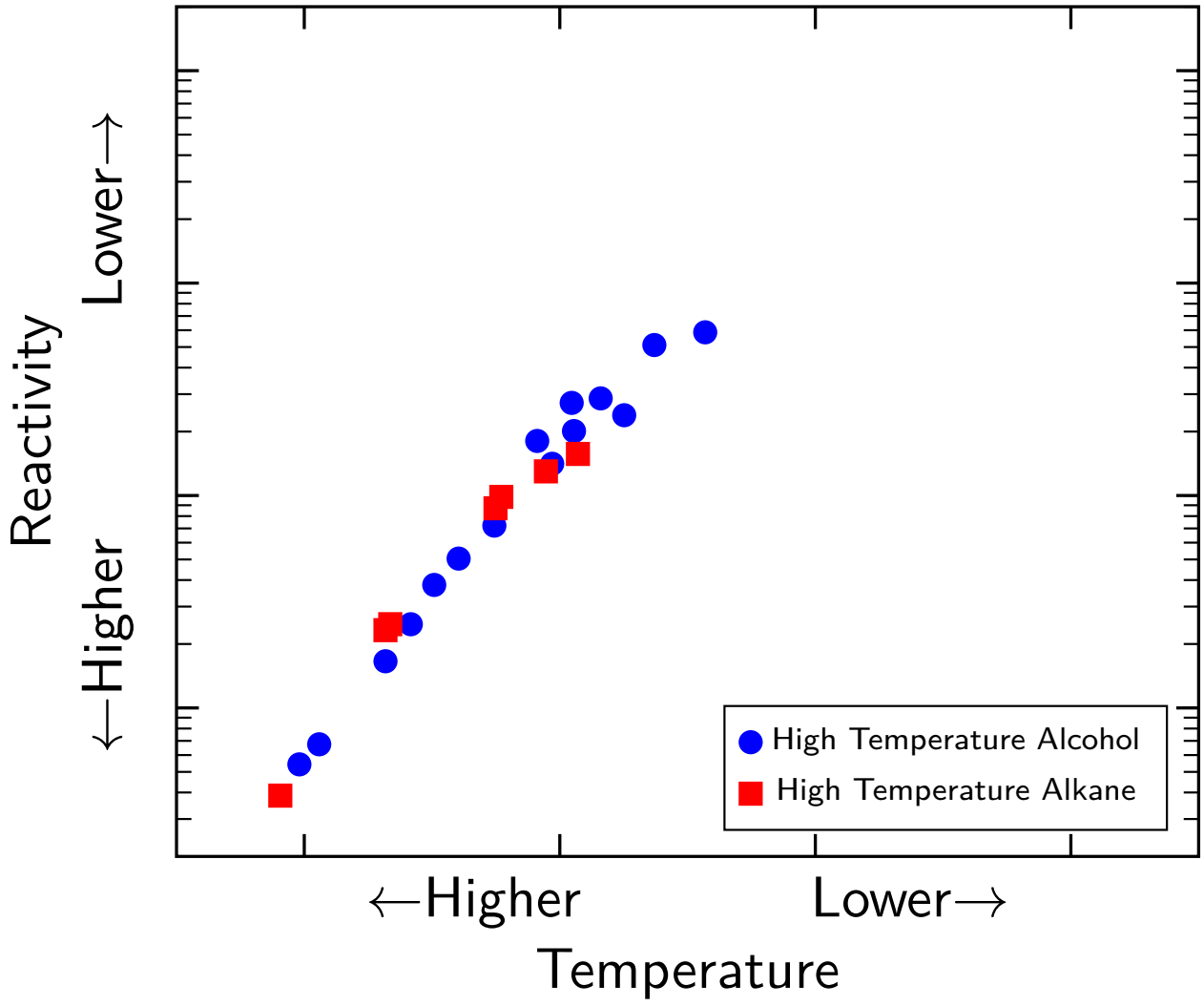

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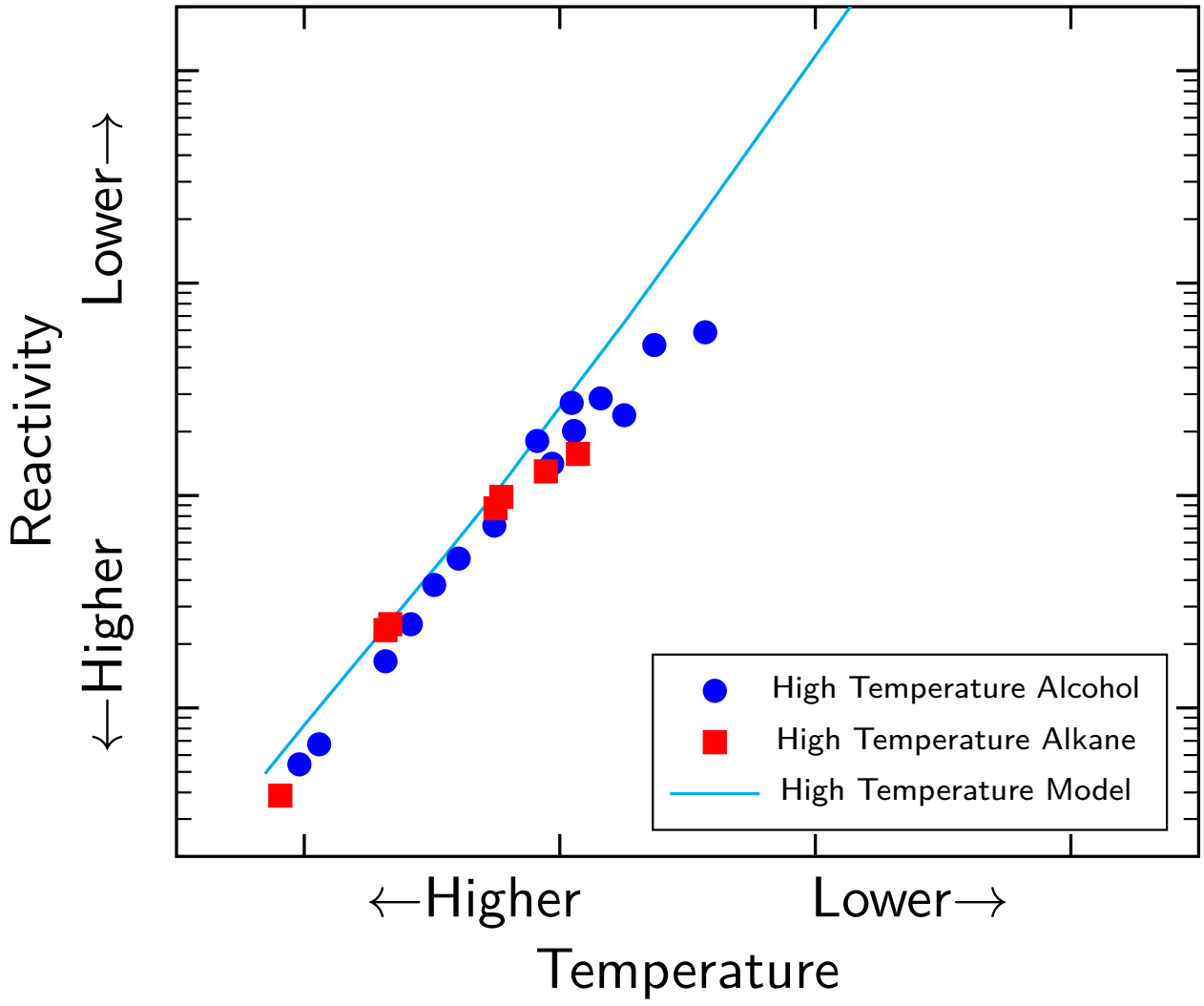

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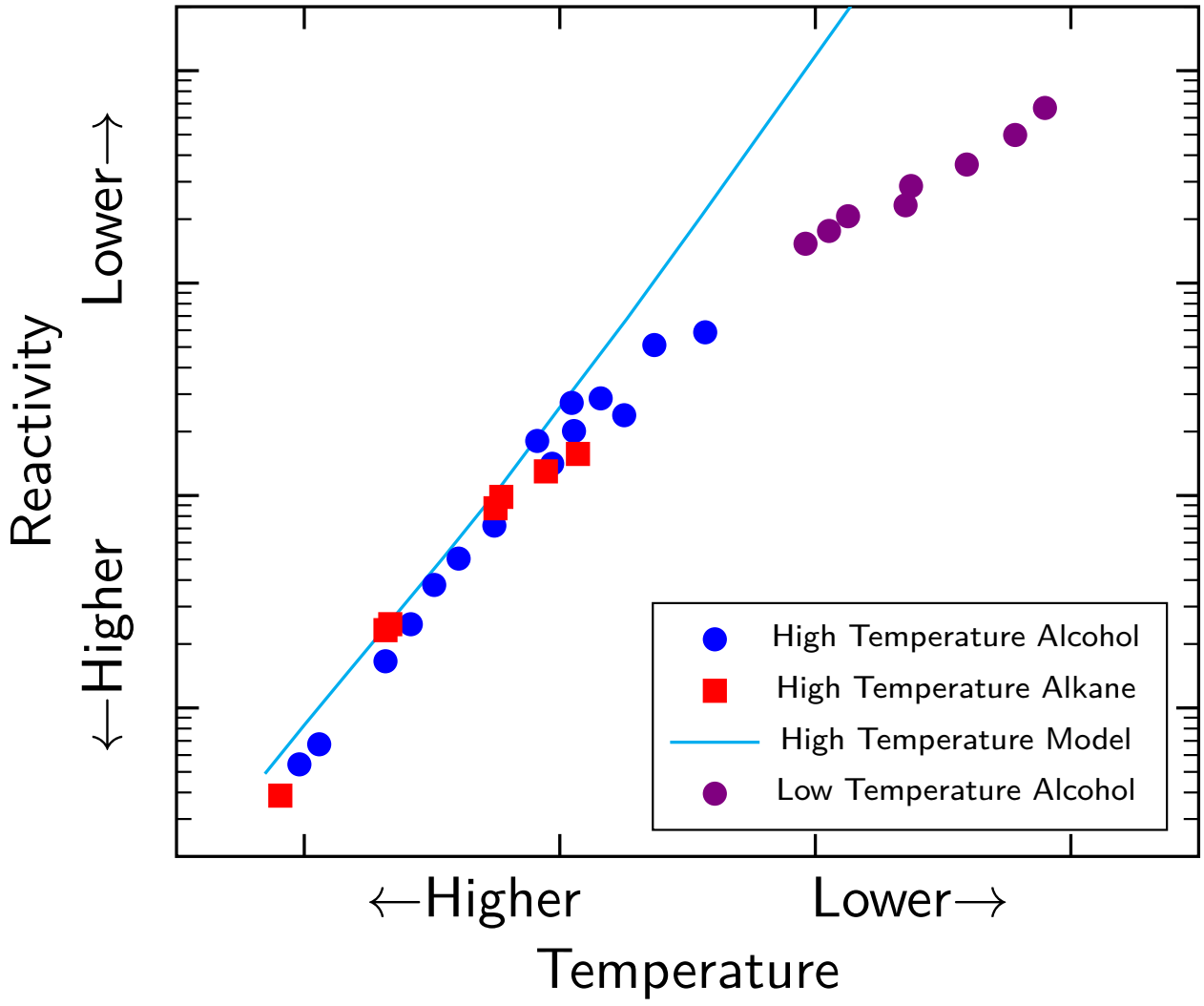

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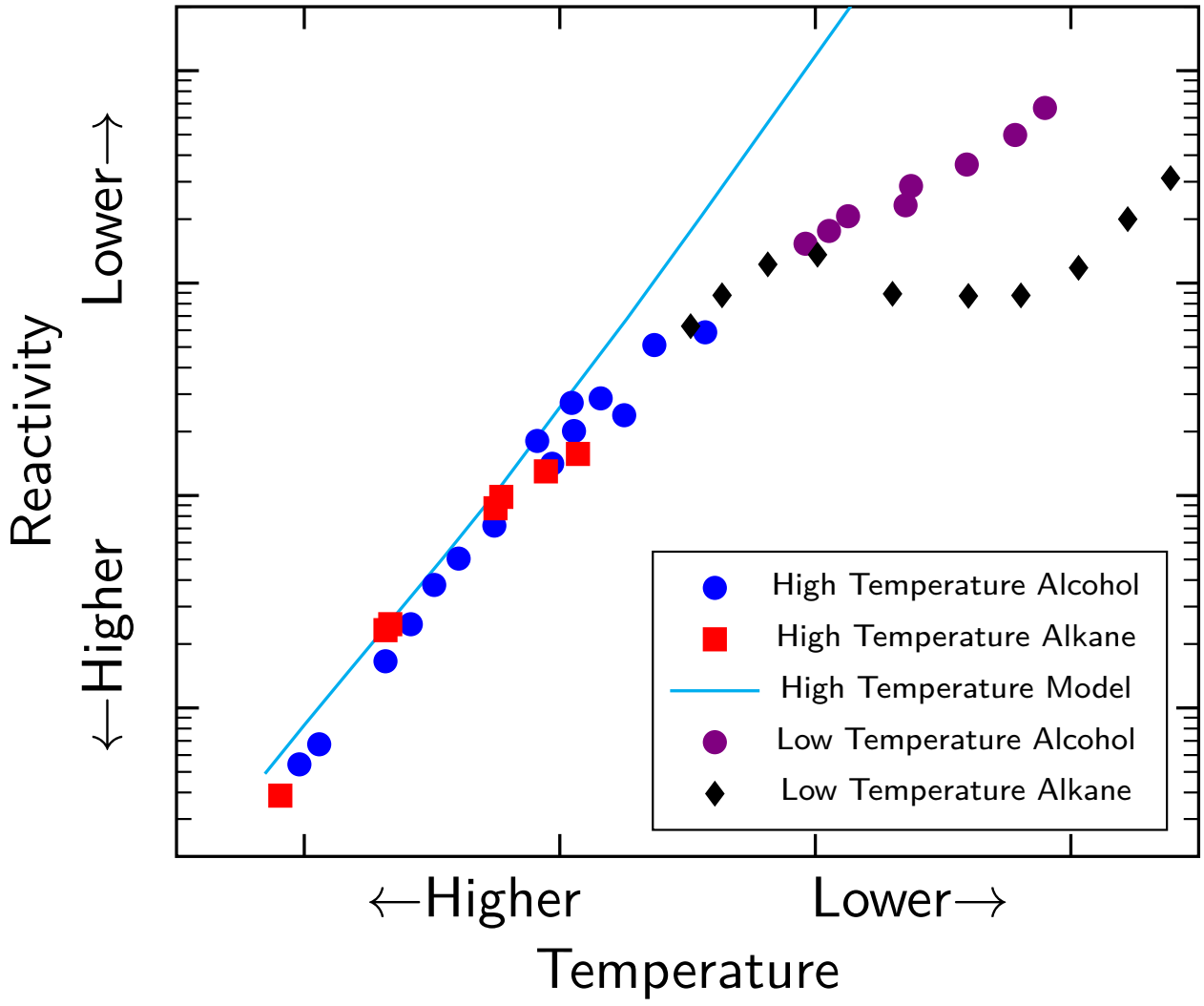

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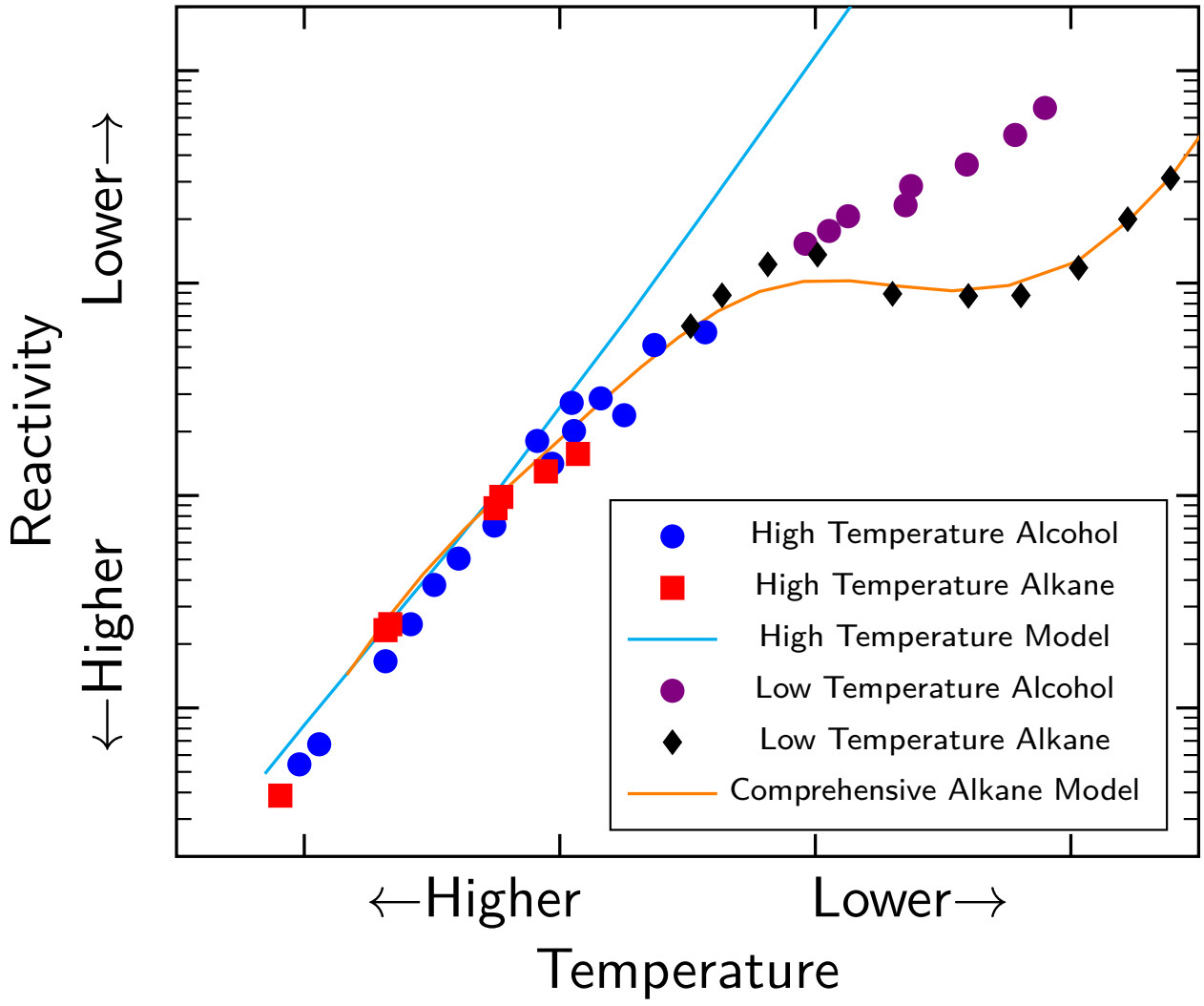

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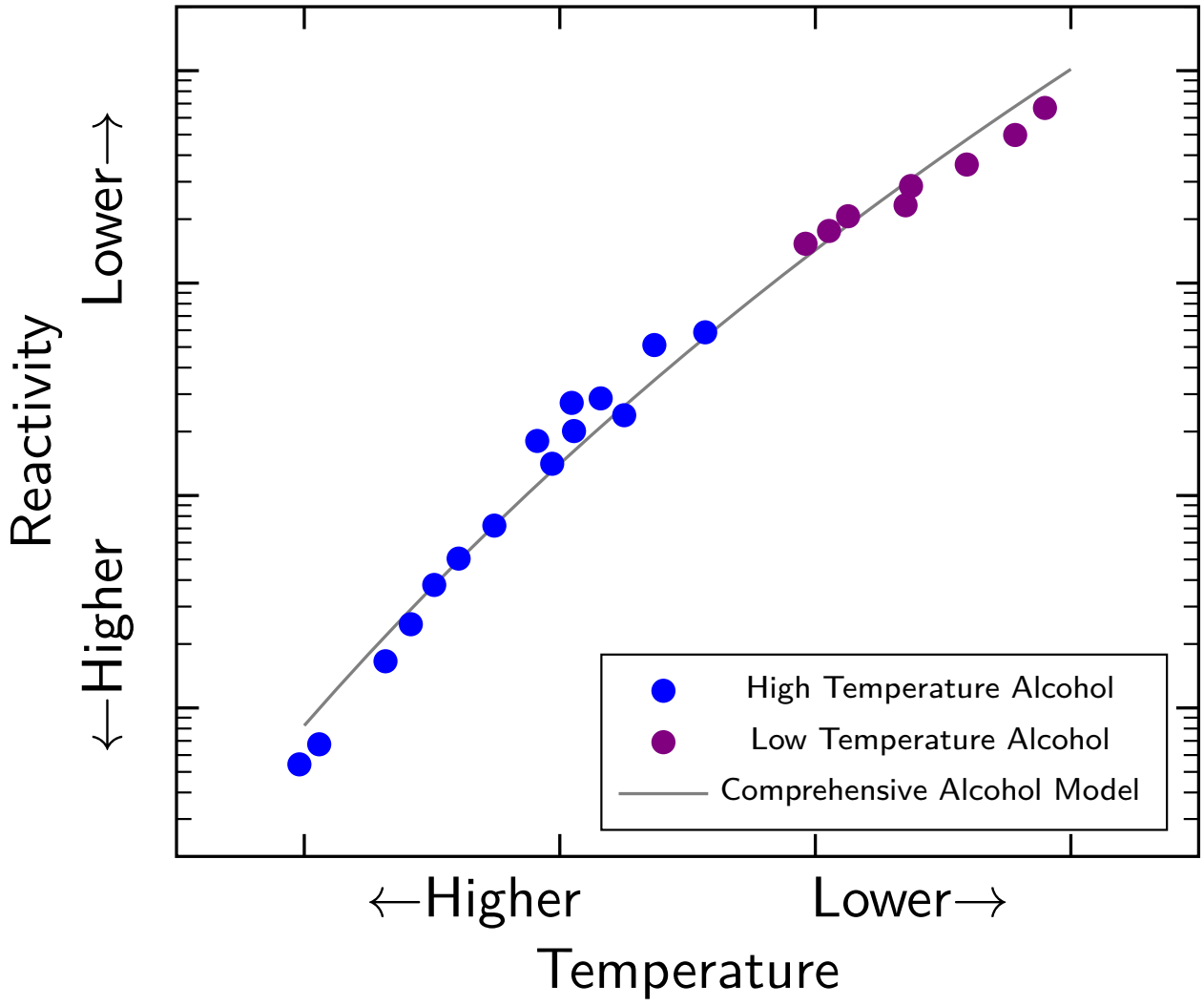

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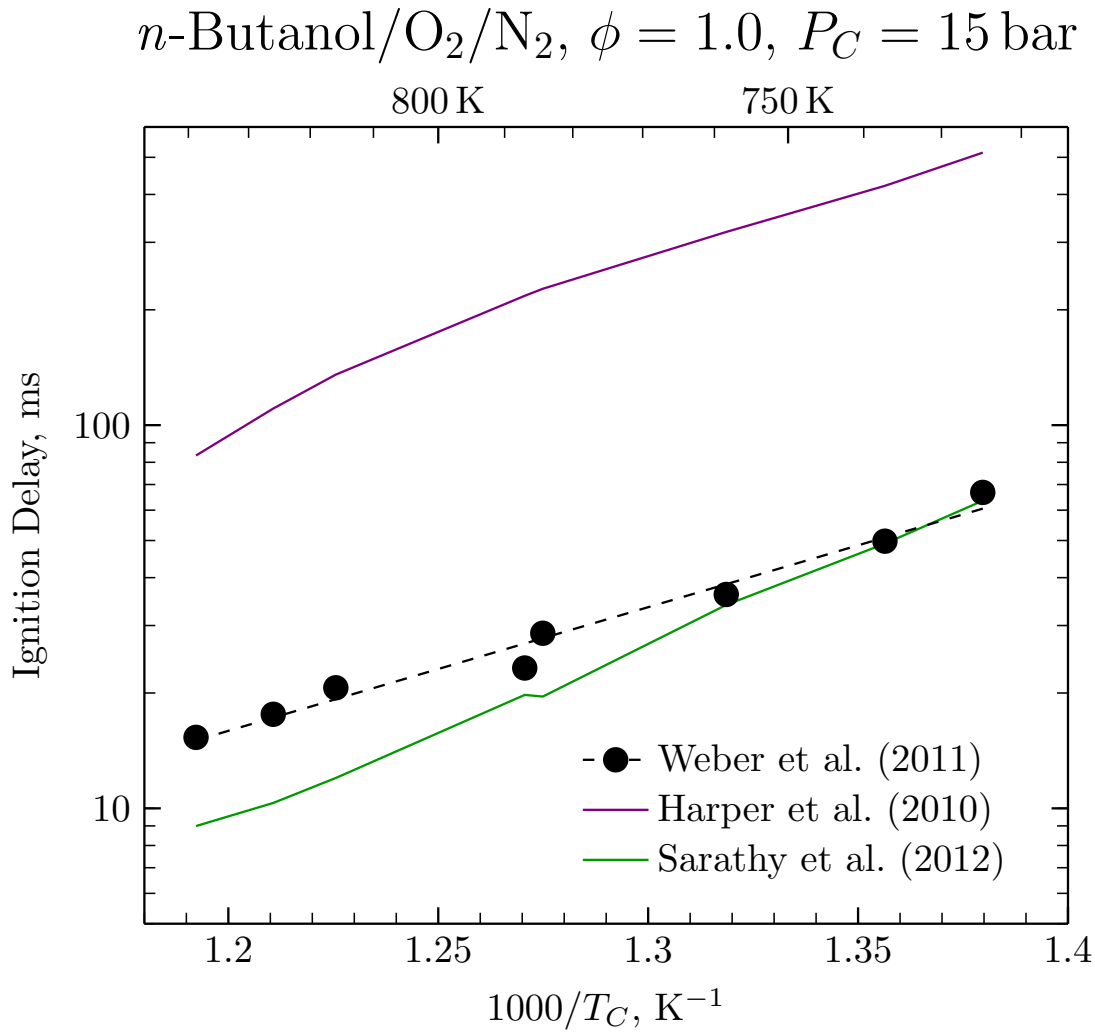

With low-temperature reaction classes added, models can better predict the ignition delay.

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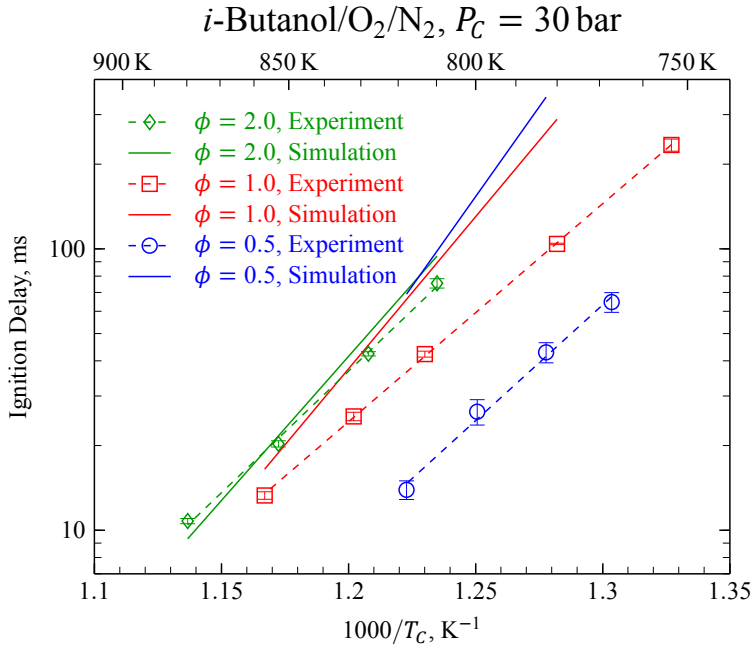
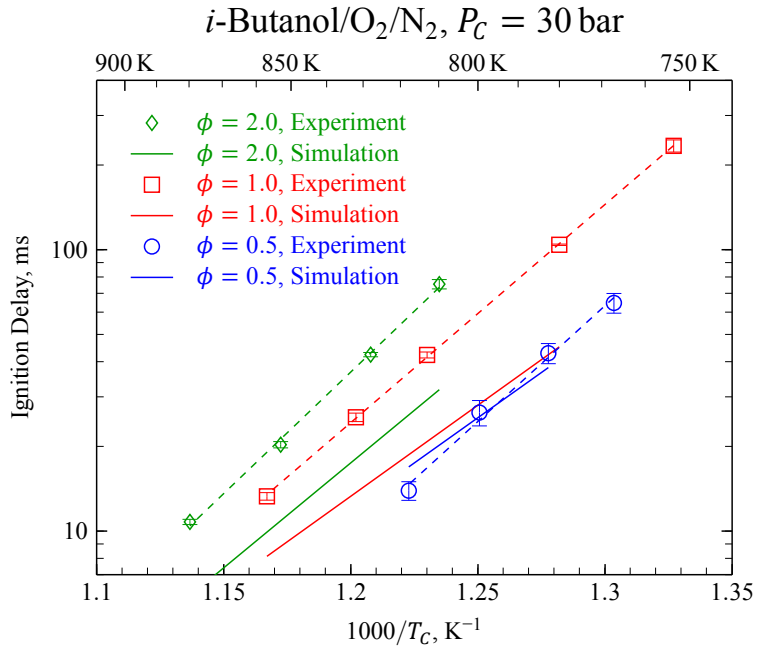


Weber et al. 8th US National Combustion Meeting 2013

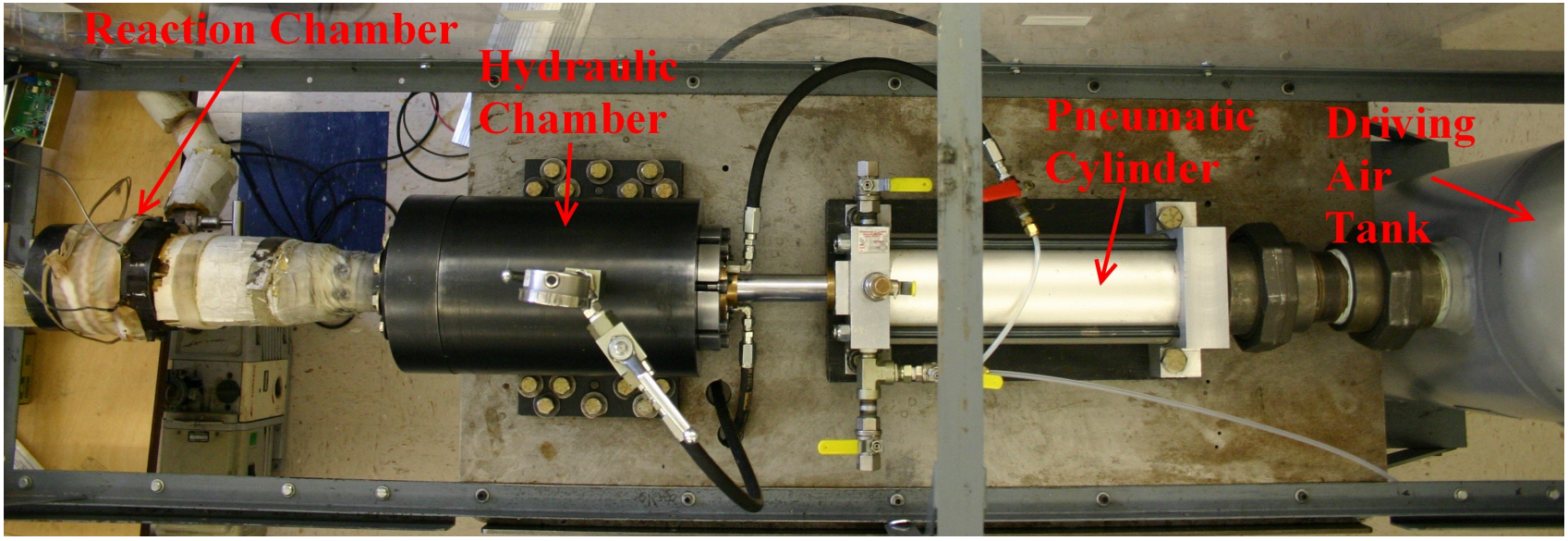


Sarathy et al. Combust. Flame 2012

There is still some critical information missing from our understanding of high-pressure, low-temperature ignition of alternative fuels

Experimental Apparatuses

Rapid Compression Machine



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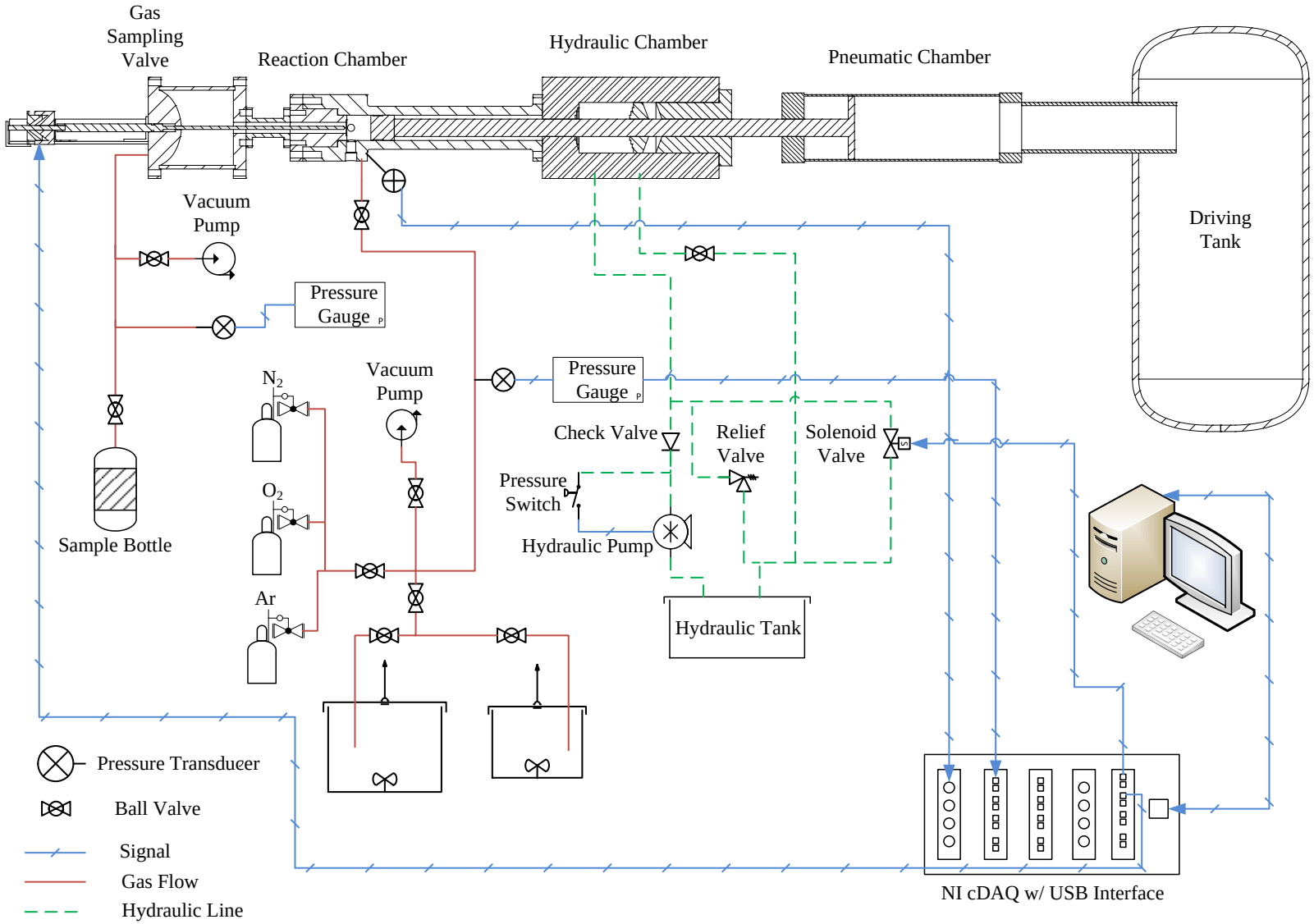
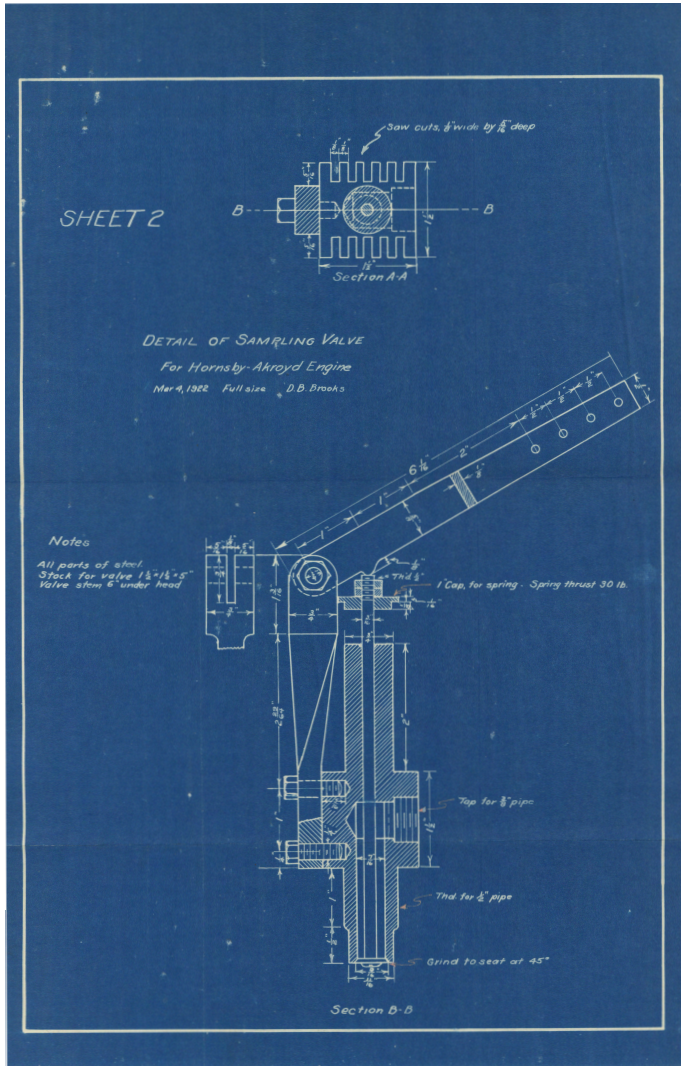


Rapid Sampling Apparatus

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



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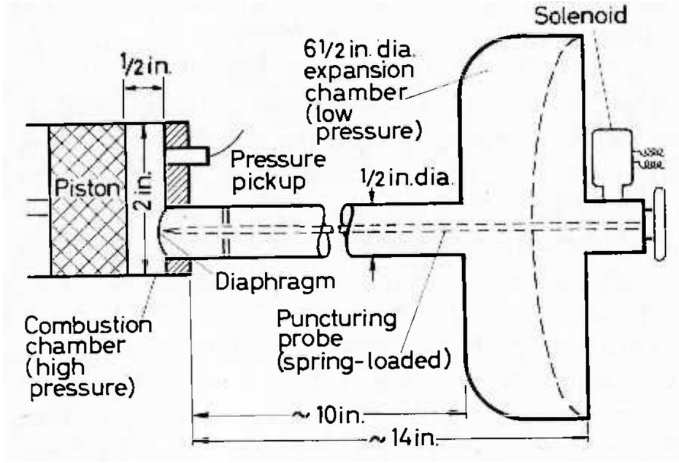

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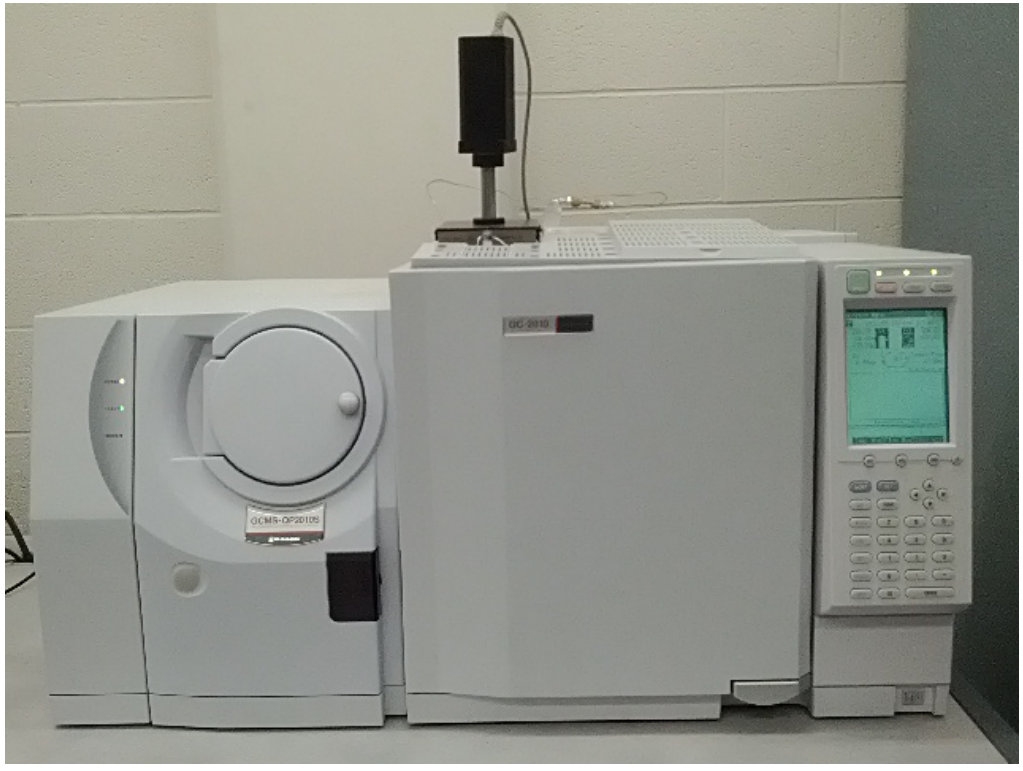
- In the 1960's, the first sampling apparatus was adapted for an RCM
- Mittal developed a similar system for the present RCM based on deactivating an electromagnet
- I have modified the design of Mittal to incorporate a solenoid instead of the electromagnet

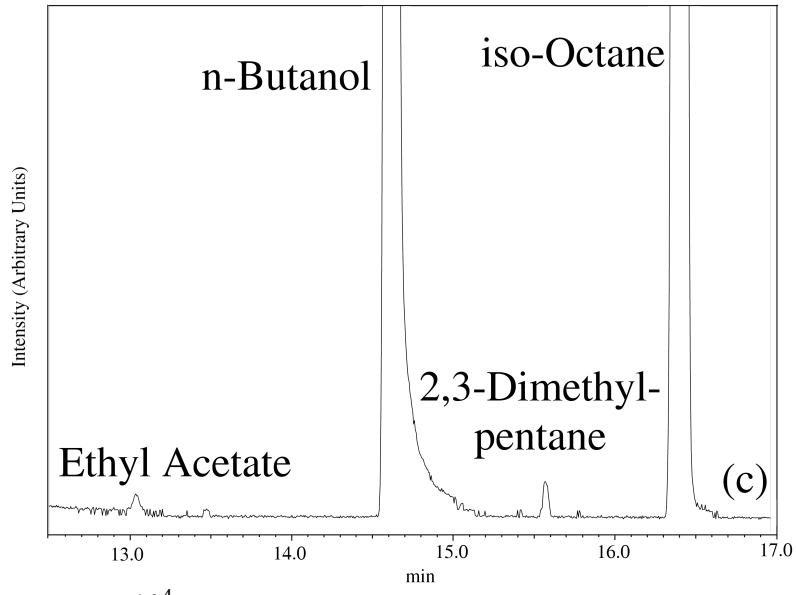
Gas Chromatograph/Mass Spectrometer

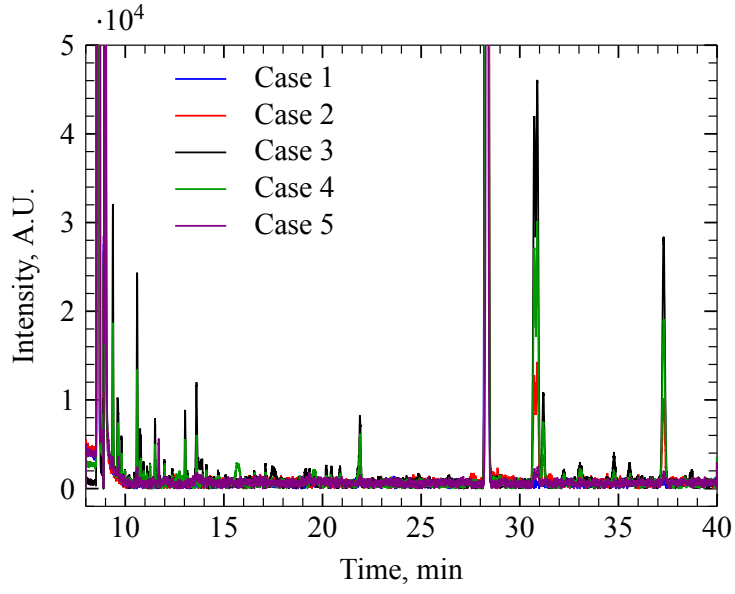
- Standard piece of chemistry lab equipment, commercially supplied (Shimadzu)



Gas Chromatograph/Mass Spectrometer

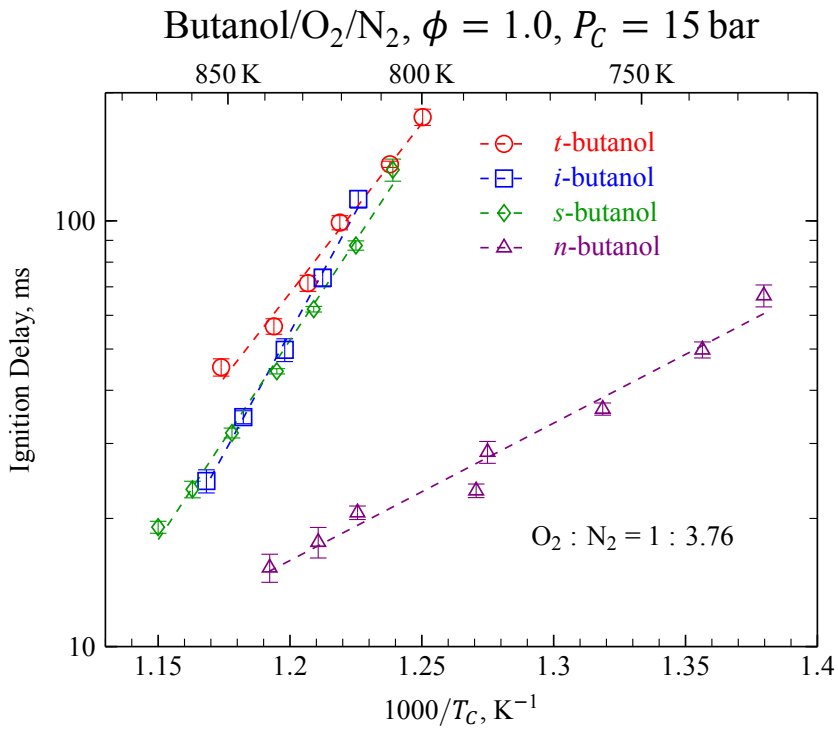
- Separates, identifies, and quantifies chemical species

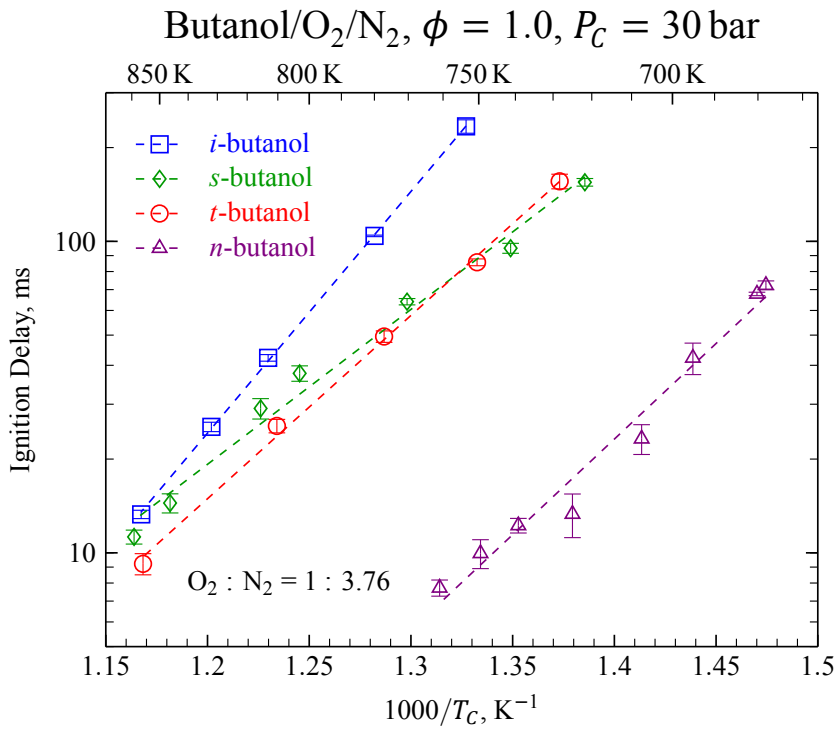




Results

The reactivity of the butanol isomers depends on the pressure





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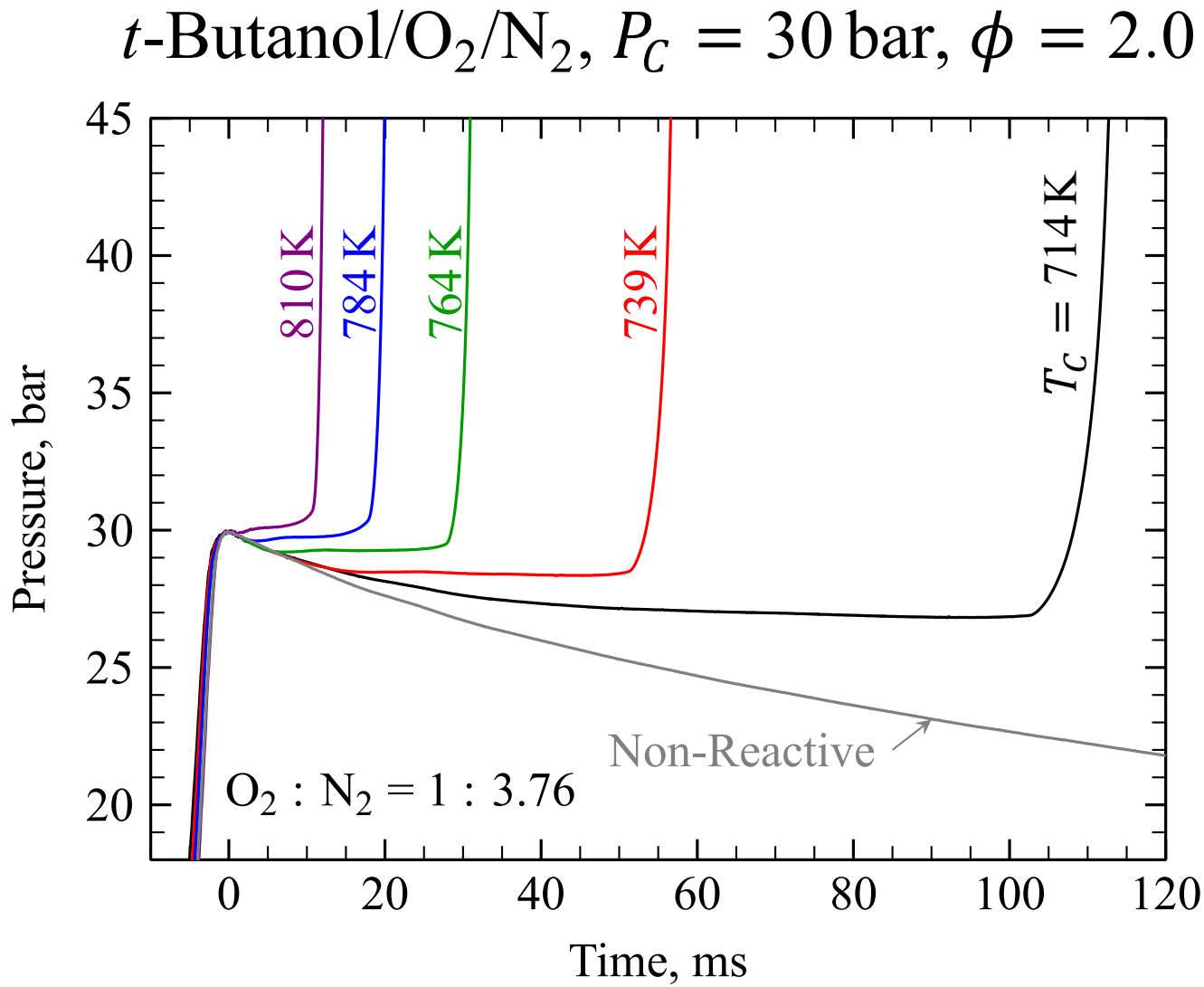
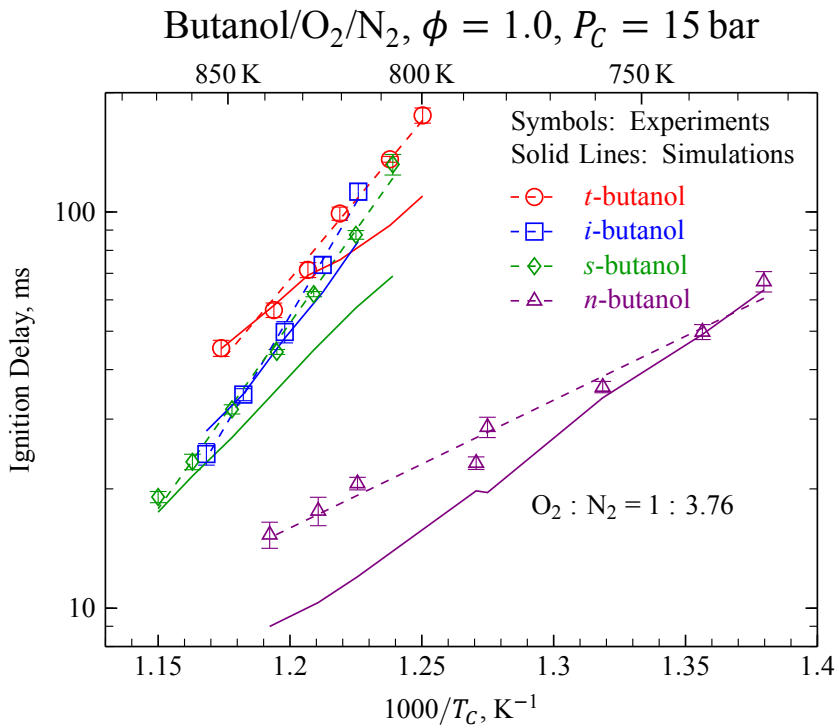
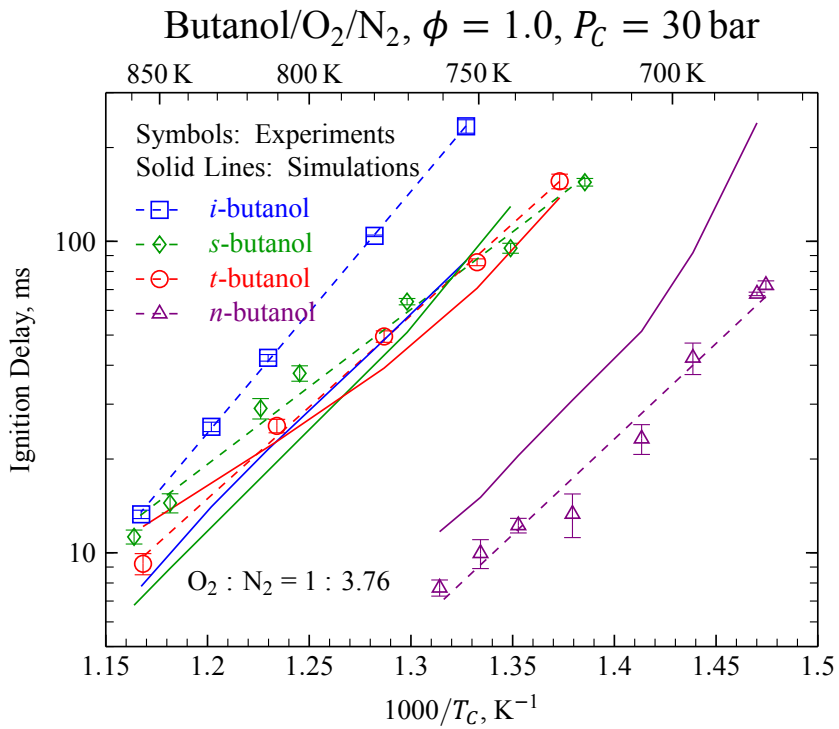


The reactivity trend can be predicted by a detailed understanding of the chemistry





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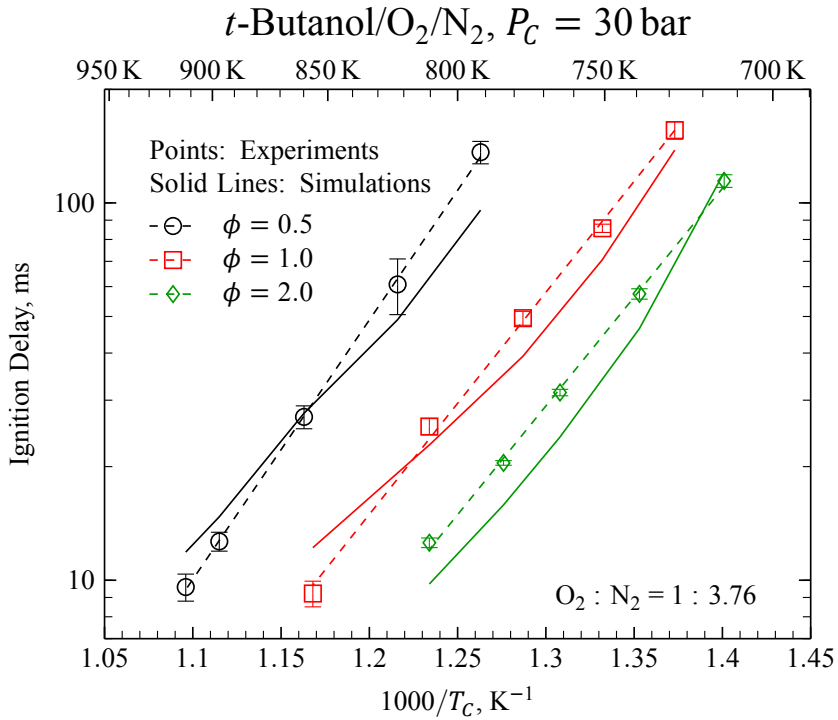
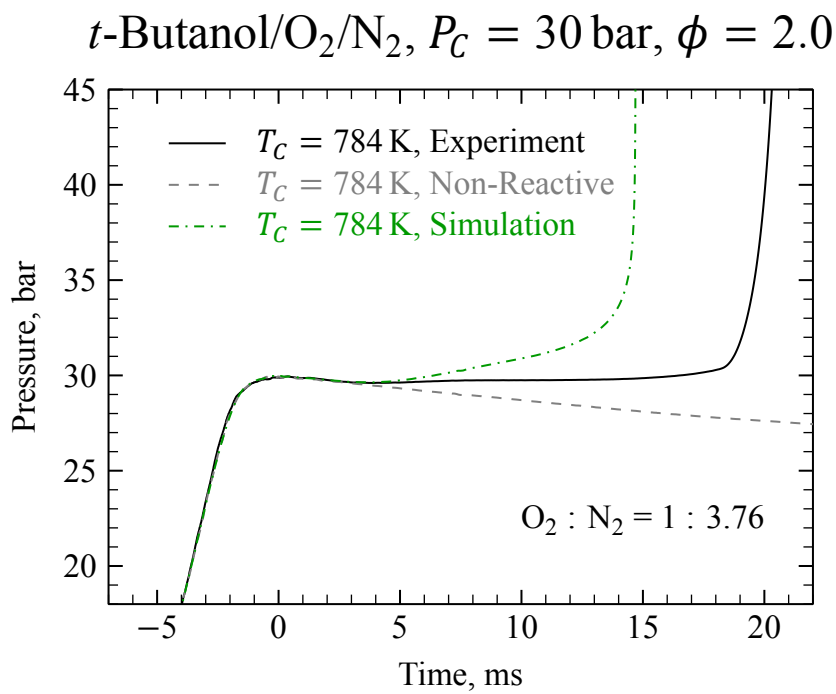
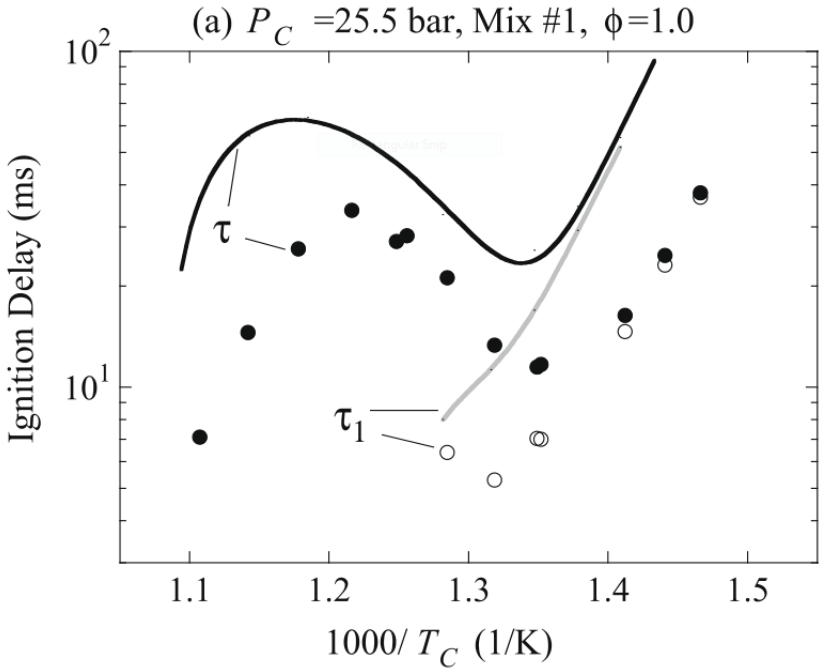
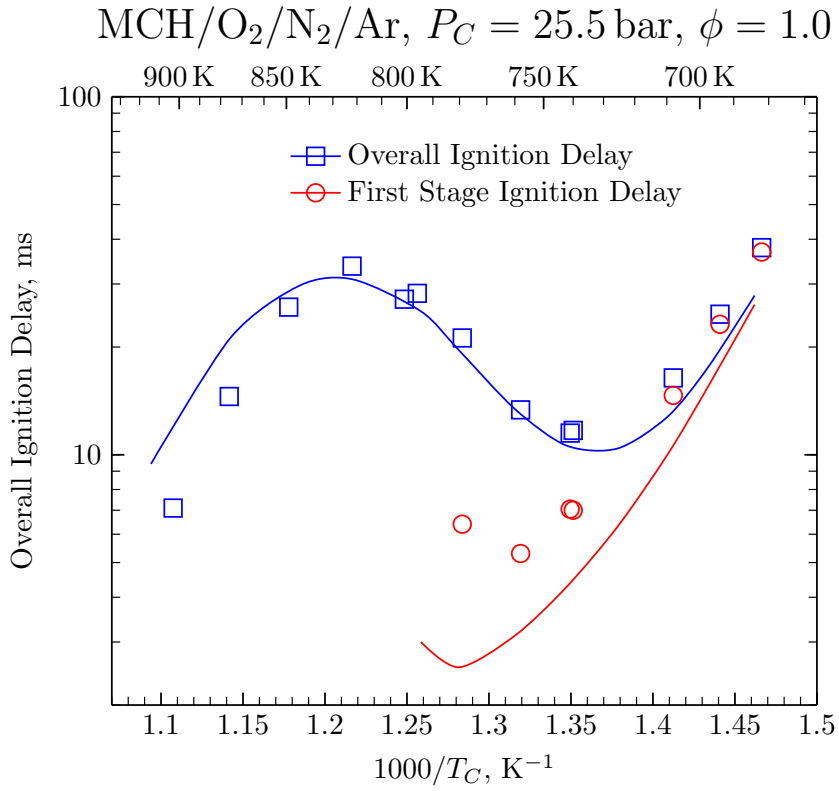




My work has lead to substantial improvements in models for hydrocarbons



Mittal et al. Combust. Flame 2009



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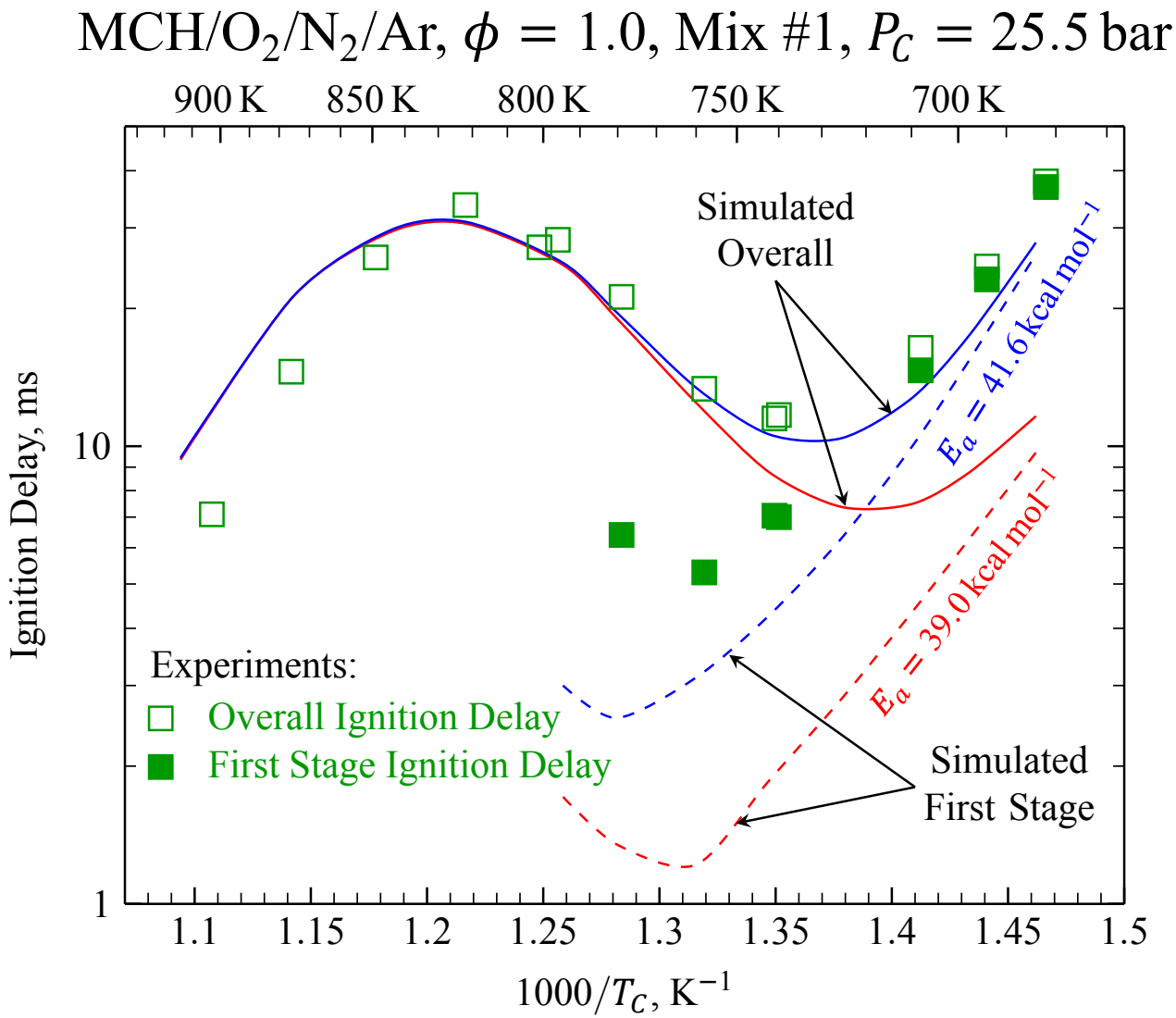
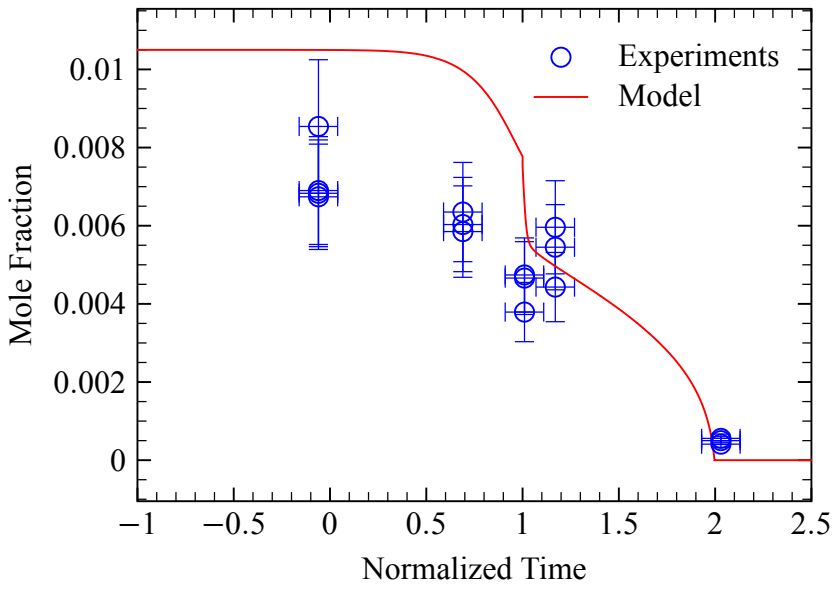
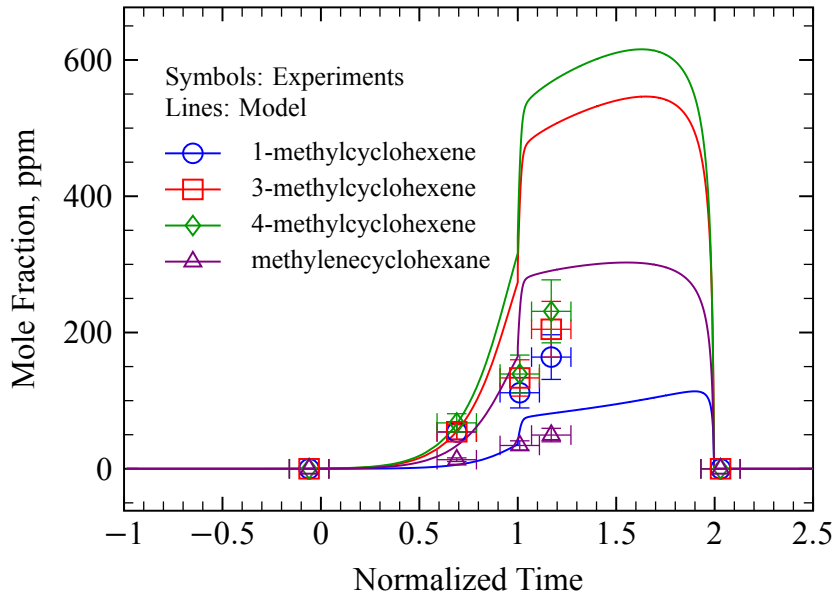


UCONN COMBUSTION DIAGNOSTICS LABORATORY

Sampling results





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