The Frontiers of Biofuel Combustion Research

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Acknowledgements
Our Pale Blue Dot

picture taken from nasa.gov
This is what it will take to reduce our dependence on fossil fuels. How many years until we are here? 50? 150?

Fossil Fuels
(70-90% going to HK buildings)
What are our options?

70 MW Kagoshima Nanatsujima Mega Solar Power Plant (started this week)


Credit: www.energy.gov
What are our options?

If we could cover Central and Kowloon with solar panels:
\[ \sim 85,000 \text{ MW} \]

Compare to the \( \sim 8000 \) MW currently coming from CLP Power and HKE*

*Information Services Department, Water Supplies Department http://www.wsd.gov.hk/
The role of combustible energy sources

Why fossil fuels continue to be used:
1) Accessible and cheap
2) High energy density

Tesla Model S battery: ~ 1 MJ/kg
Ford Model T gasoline engine: ~ 50 MJ/kg

Why Hong Kong needs an energy source like hydrocarbons:
1) Building functions (e.g., AC, lighting, stoves)
2) Backup power generation. Largest gasoline generators almost the size of average Hong Kong apartment
3) There are still a lot of [older] cars

*pictures form Tesla and the Antique Automobile Club of America*
The Holy Grail: Carbon Neutral Fuels
Alternative and Biofuel sources

Fossil Synfuels
- Gas-to-Liquids (GTL)
- Tar-sand-to-Liquids (TSTL)
- Coal-to-Liquids (CTL)
- Coal/Biomass-to-Liquids (CBTL)
- Coal-to-Syngas

First Generation Biofuels
- Sugar/corn to Ethanol, Butanol
- Oil/fat Biodiesel

Second Generation Biofuels
- Non-food plants (Algae, Jatropha) To Liquid
- Cellulose-to-Liquids
- Lignocellulosic Biomass-to-Liquids

Solar Fuels
- Electrolysis of H₂
- Artificial Photosynthesis

With so many possibilities, combustion scientists are needed to ensure proper integration of fuel candidates.
Overview of the CEFRC

Our Goal: development of validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines and of future fuels themselves

- 8 academic institutions and 2 national laboratories
- Foci:
  - H_2/CO, small hydrocarbons (syngas) are the foundation of larger fuels
  - Butanol and biodiesel constitute most Biofuels
Multi-scale modeling describes combustion processes, from quantum scales up to device-level, continuum scales.
Teams Can Move Fast

• In less than 2 years, went from zero to good model for butanol combustion, validated by many different types of experiments
• Contrast: sequential single-investigator model-building and comprehensive validation usually takes decades.
• Pre-publication sharing of data and results
Butanol: CEFRC’s First Test Case

- Butanol is about to be commercialized
- Butanol has advantages over ethanol
  - More soluble in gasoline
  - Can be used at higher blending ratios (above 10%)
  - Can be shipped in gasoline pipelines
  - Lower vapor pressure: less smog
  - No engine modifications needed
  - Higher energy density

A great candidate as an alternative fuel or fuel additive for ground transportation and backup energy generation
Butanol: The Methodology

- Create a butanol model and a foundation model
- Identify conditions where experiments are needed and carry them out
- Compare model predictions with experimental data
What are Foundational Fuels?

Initial fuel cracking is decoupled from the subsequent kinetics of the cracked products\(^1,2\)

\(^1\)X. You; F. N. Egolfopoulos; H. Wang, Proceedings of the Combustion Institute 2009

\(^2\)C. Ji; E. Dames; B. Sirjean; H. Wang; F. N. Egolfopoulos, Proceedings of the Combustion Institute 2011
Typical combustion kinetic mechanism for large fuels consists of:

- Hundreds of species
- Thousands of reactions

Rate parameters determined by:

- experiments
- quantum chemistry & reaction rate theory
- analogues
The shock tube is an ideal reactor for studying chemical kinetics:
- Constant volume, constant internal energy, stagnant gas
  - Heat transfer, bulk gas flow, and turbulence are negligible
  - Only relevant physical phenomenon is chemical reactions
Example Data: Methanol

Ren, Dames et al., *Combust. Flame*, 2013
Example Data: Methanol

Ren, Dames et al., Combust. Flame, 2013
Important Combustion Phenomena Sensitive to Chemistry, Mixing, Flows

\[
\begin{align*}
\log \chi & \quad \xi & \quad \text{OH} & \quad \text{HO}_2 & \quad \text{CH}_2\text{O}
\end{align*}
\]
Conclusions

• The world’s megacities must utilize combustible fuels for decades to come
• Combustible fuels will play an important role far into the future
• Current and future efforts will enable near carbon neutral fuels