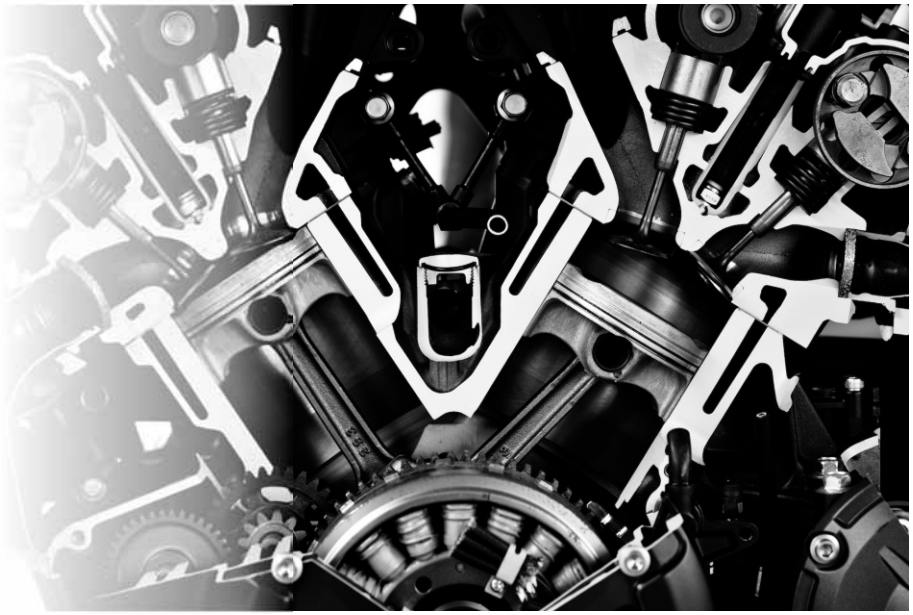
COMBUSTION RESEARCH FACILITY

What Do Engines Want for Breakfast?

Charles J. Mueller
Combustion Research Facility
Sandia National Laboratories

Sustainable Transportation Summit
Walter E. Washington Convention Center
July 12, 2016

Outline

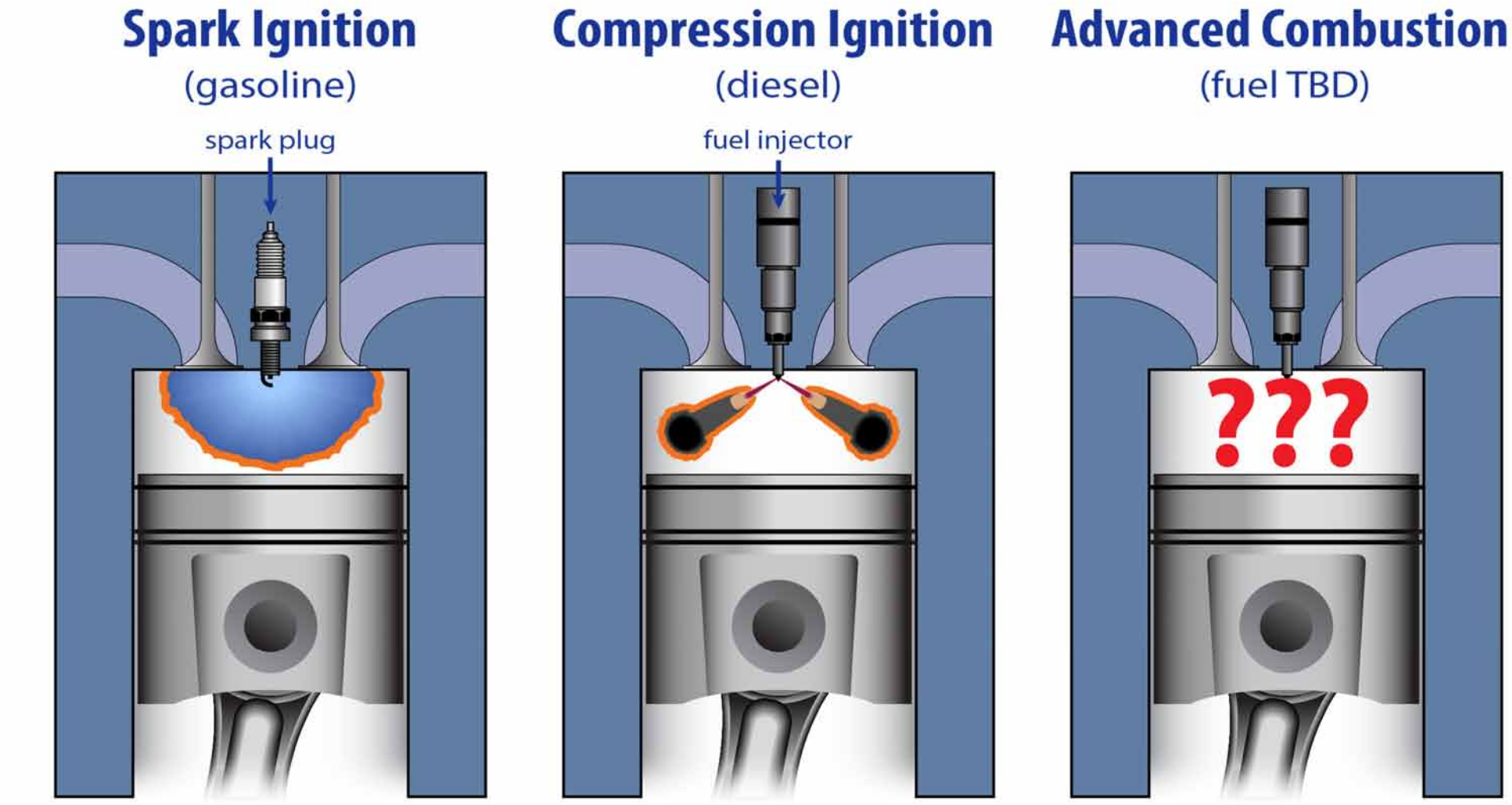


- **Classes of reciprocating engines**
  - Spark ignition
  - Compression ignition
  - Advanced combustion
- **Classes of fuel properties**
  - Chemical and physical
  - Environmental and consumer acceptance
  - Production and distribution

- **Key fuel properties from an engine perspective**
  - Ignition quality
  - Volatility
  - Composition
- **Property guidance for different engine types**

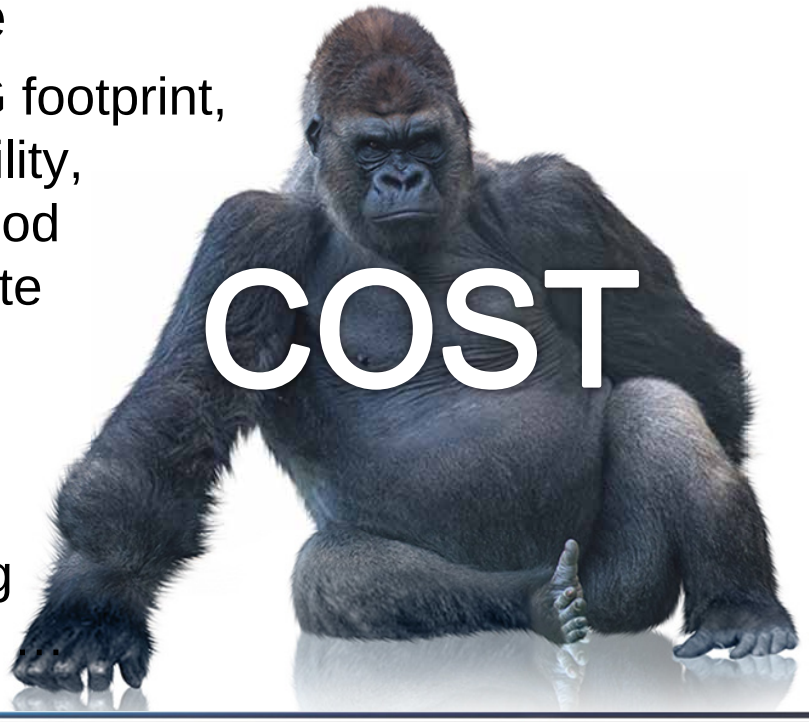
Classes of Reciprocating Engines

- There are three primary classes of ground-vehicle engines



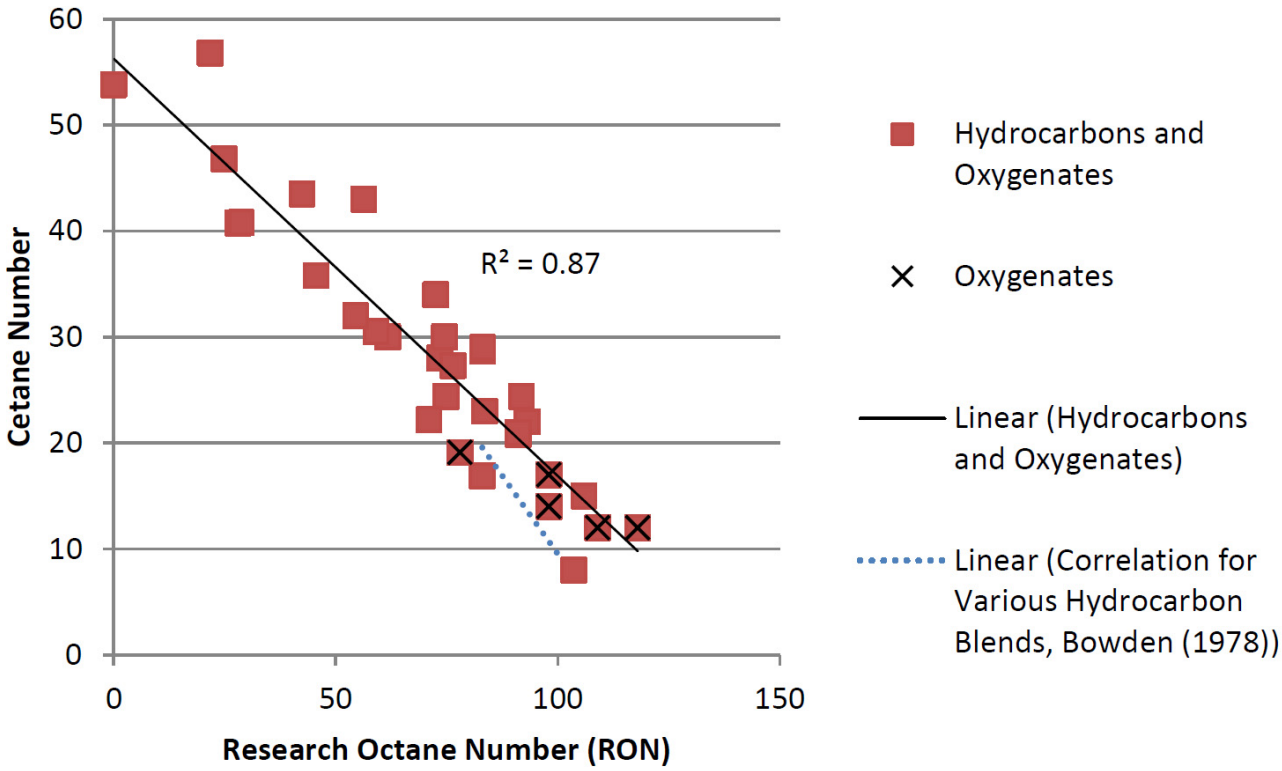
Classes of Fuel Properties

- **There are also three main classes of fuel properties**
  - Chemical and physical ← most important from the engine's perspective
    - Ignition quality, volatility, composition, energy content, density, cold-flow performance, corrosivity, oxidative stability, solubility (of renewable component[s] in base fuel), water tolerance, elastomer compatibility, viscosity, lubricity, electrical conductivity, & surface tension
  - Environmental and consumer acceptance
    - Toxicity (acute, chronic, reproductive), GHG footprint, toxic emissions, sustainability, biodegradability, backward compatibility with existing fleet, food vs. fuel, indirect land-use changes, odor/taste thresholds, …
  - Production and distribution
    - Scalability (market for "by-products"?), product variability, compatibility with existing distribution infrastructure (e.g., pipelines), & …



Ignition Quality

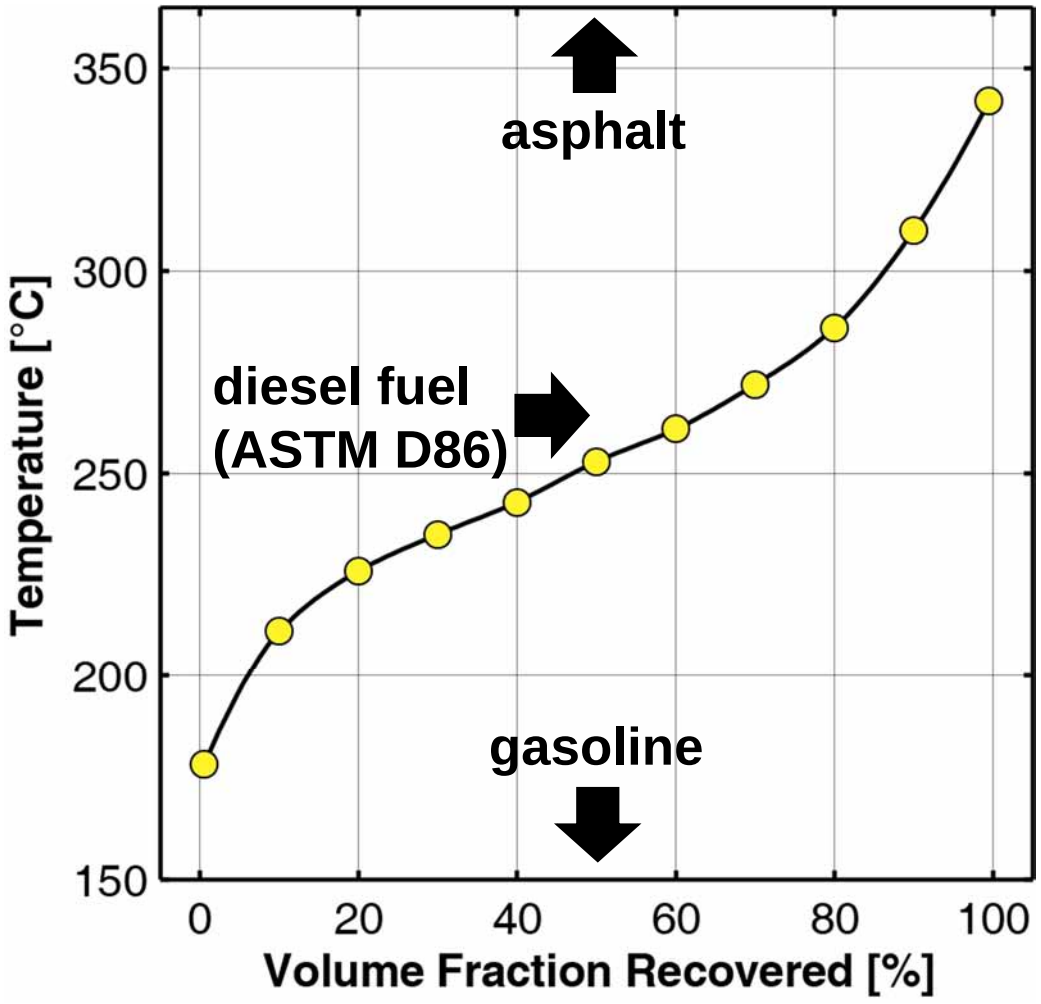
- **How easy is it to ignite a fuel/charge-gas mixture?**
- **Ignition quality is arguably the most important fuel property from a combustion standpoint**
- **Metrics**
  - Cetane Number (CN)
  - Research / Motor Octane Number (RON / MON)
  - Sensitivity (S = RON – MON)
  - Flammability limits
  - Flame speed
  - Tolerance to EGR
  - Minimum ignition energy



Source: J. Yanowitz et al., "Compendium of Experimental Cetane Numbers," NREL/TP-5400-61693, August 2014.

Volatility

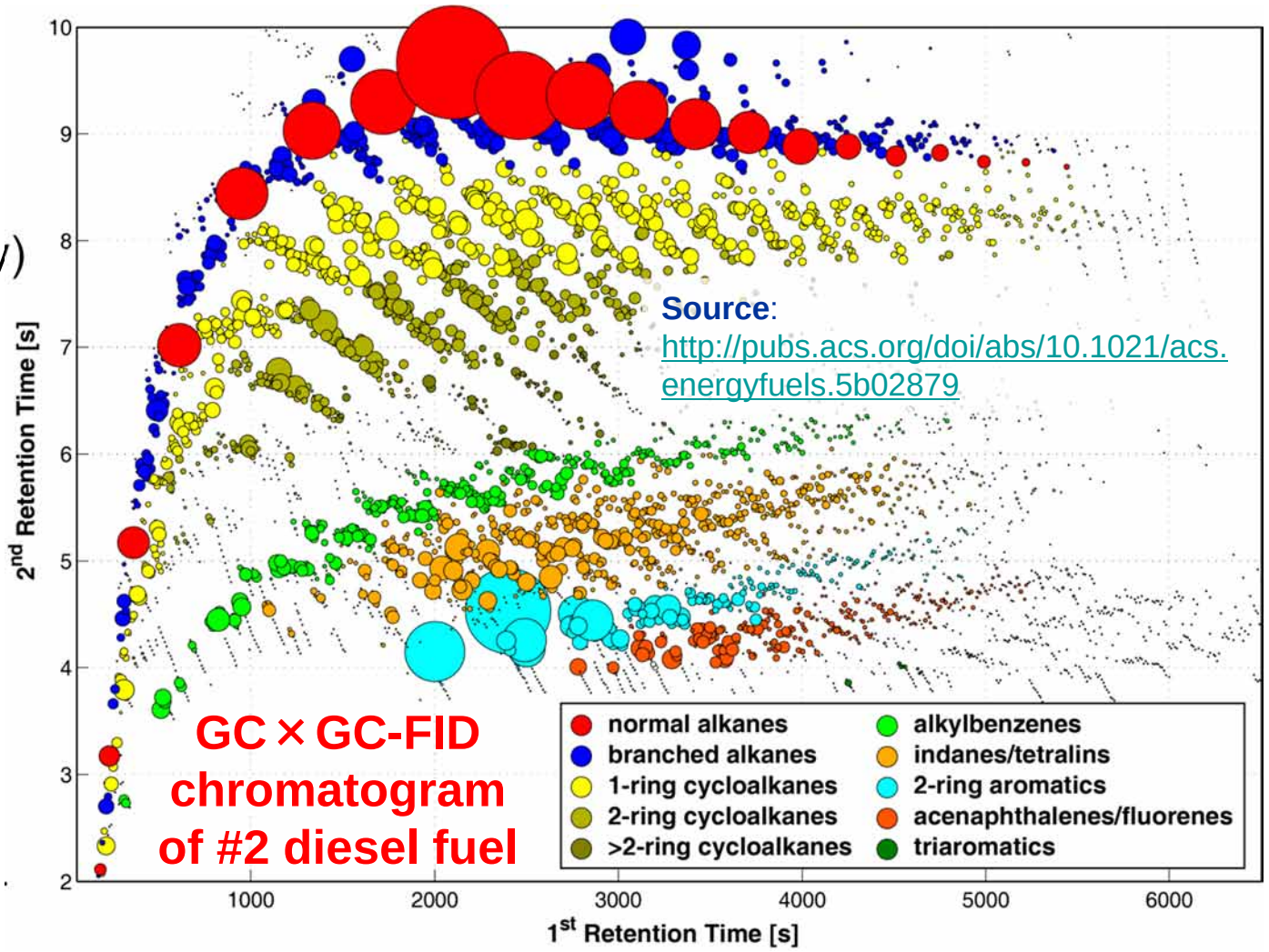
- **How readily does the fuel change phase from liquid to vapor?**
- **Metrics**
  - Boiling point /distillation curve
  - Flash point
  - Liquid heat capacity
  - Heat of vaporization (HoV)
  - Vapor pressure



Source:
http://pubs.acs.org/doi/abs/10.1021/ef300303e

Composition

- **What kinds of atoms and molecules are present in the fuel?**
- **Metrics**
  - Elemental analysis
    - C, H, O, N, S, P, metals (alkali, heavy)
  - Molecular analysis
    - Hydrocarbons
      - Normal, branched, and cyclic alkanes
      - Alkenes
      - Aromatics
    - Oxygenates
      - Alcohols, esters, ethers, ketones, furans, aldehydes,…
    - Water



COMBUSTION RESEARCH FACILITY

Fuel-Property Guidance

Fuel-Property Guidance for SI Engines

- **Co-Optima developed a merit function to quantify Δ in engine efficiency due to fuel-property Δs**

$$Merit = \sum \boxed{\frac{(RON_{mix} - 91)}{1.6}} - \boxed{K\frac{(S_{mix} - 8)}{1.6}} + \boxed{\frac{(S_{L\,mix} - 46[cm/s])}{3}}$$

RON | Octane Sensitivity | Flame Speed

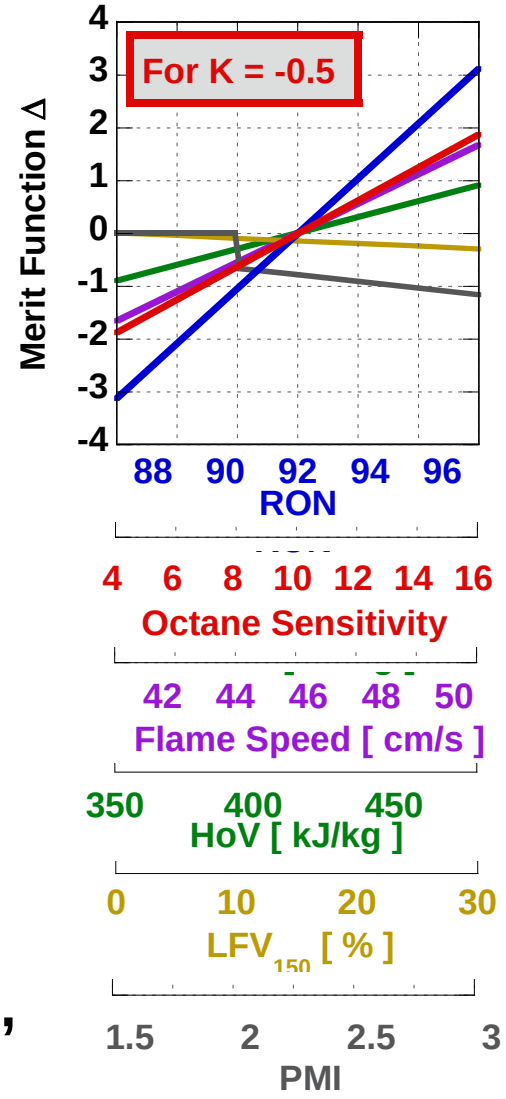
$$+ \boxed{\frac{0.01[ON/kJ/kg](HoV_{mix} - 415[kJ/kg])}{1.6} + \frac{(HoV_{mix} - 415[kJ/kg])}{130}}$$

Heat of Vaporization

$$- \boxed{LFV_{150}} - \boxed{H(PMI - 2.0)[0.67 + 0.5(PMI - 2.0)]}$$

Distillation | Particulate Matter Index (PMI)

Source: Paul Miles, SNL



Source: Jim Szybist, ORNL

- **Hence, want fuel to meet all current gasoline specs, plus have RON > 91, S > 8, S_L > 46 cm/s, HoV > 415 kJ/kg, all fuel boiling below 150 °C, and PMI < 2**

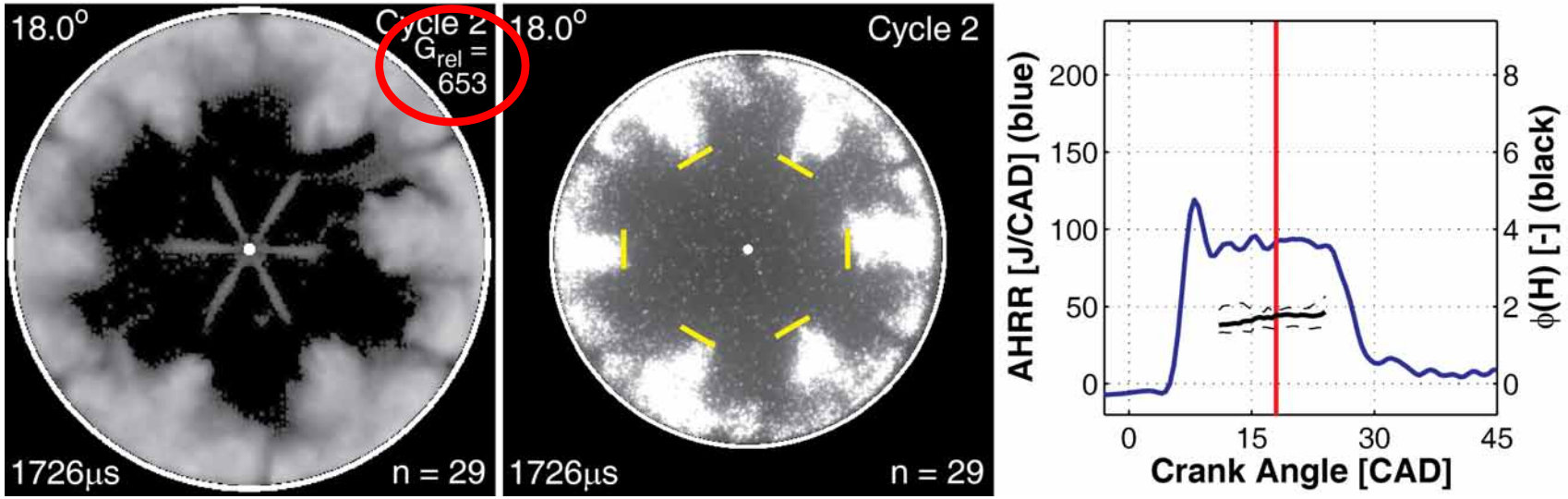
Fuel-Property Guidance for CI Engines

- **In general, today's diesel fuel specification is a good bogey**
- **Proposed targets:**
  1. Cetane number (CN) required > 40 (> 55 if possible)
  2. Volatility such that the headspace in a fuel storage tank will not be explosive (i.e., the headspace should fall either above the rich or below the lean flammability limit)
  3. Freezing point below -10 °C, and lower than -40 °C if possible
  4. Soluble in low-aromatic base fuel to -10 °C
  5. Blend does not separate into two (or more) phases in the presence of 1000 ppm of water
  6. Normal/final boiling point below 350 °C
  7. Toxicity lower and biodegradability similar to current finished gasoline and diesel fuels
  8. Corrosivity equal to or lower than those of current finished gasoline or diesel fuels
  9. Oxidative stability equal to or better than those of current finished gasoline or diesel fuels
  10. No heteroatoms beyond oxygen and possibly nitrogen (i.e., no metals, S, P, etc.)
  11. Lower heating value (i.e., net heat of combustion) of at least 25 MJ/kg
  12. Compatibility with commercially available elastomers
  13. Viscosity between ~0.5 and 5.0 cSt at 40 °C
  14. No strong odor

Fuel-Property Guidance for Advanced-Combustion Engines

- **Use guidelines on previous slide, with following modification:**
  - If CN > 40, normal/final boiling point can be up to 350 °C
  - If CN < 30, normal/final boiling point can be up to 150 °C
- **Final observation: fuel-bound oxygen can be highly beneficial for facilitating advanced, mixing-controlled combustion modes**

Natural Luminosity **OH* Chemiluminescence** **Apparent Heat-Release Rate**



Source: R.K. Gehmlich et al., "Leaner Lifted-Flame Combustion Enabled by the Use of an Oxygenated Fuel in an Optical CI Engine," *SAE Int. J. Engines* **9**(3), doi:10.4271/2016-01-0730, 2016.