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Fuel Effects on Ignition and Their Impact on Advanced Combustion Engines

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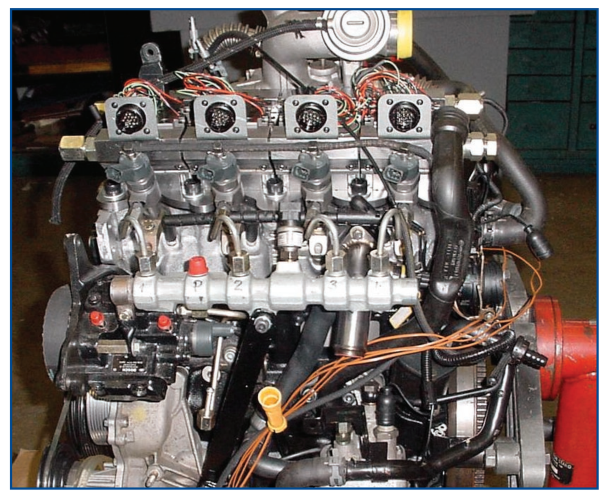
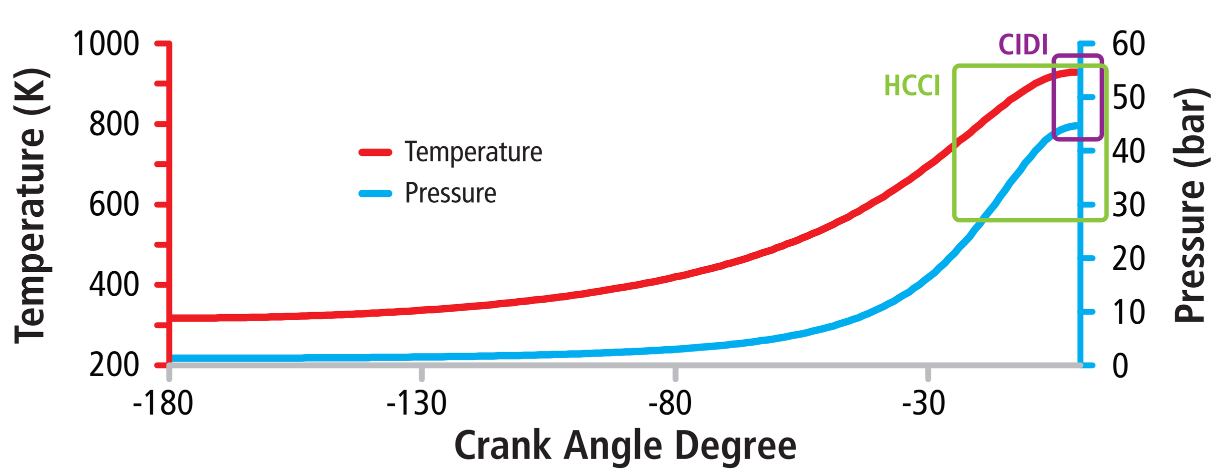
Overview

Objective

Develop a pathway to use easily measured ignition properties as metrics for characterizing fuels in advanced combustion engine research
- Correlate IQT™ measured parameters with engine data

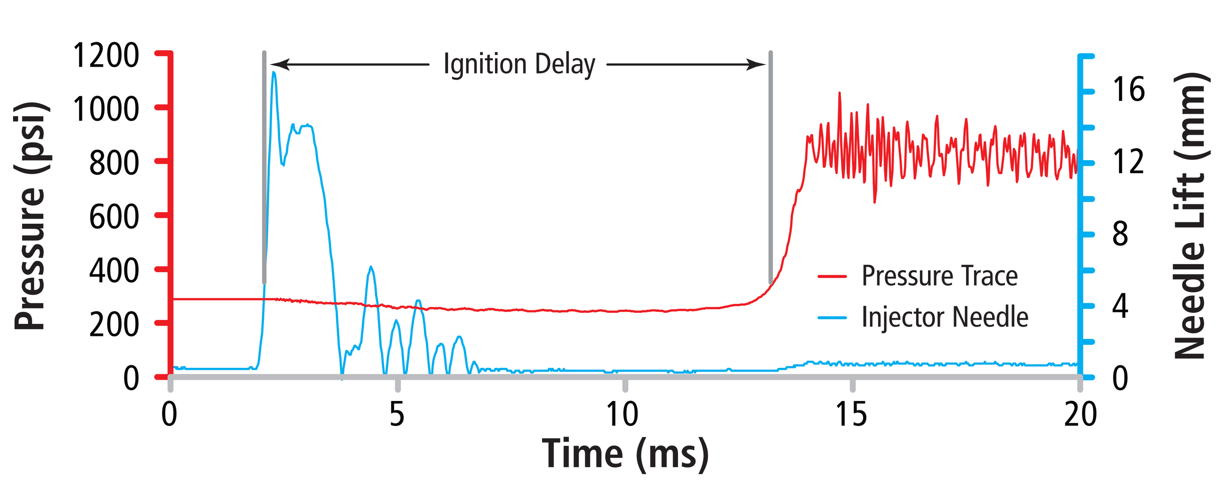


In HCCI engines, ignition timing depends on the reaction rates throughout compression stroke
- Need to understand sensitivity to T, P, and $[O_2]$
- Need to rank fuels based on more than one set of conditions
- Need to understand how fuel composition (molecular species) affect ignition properties



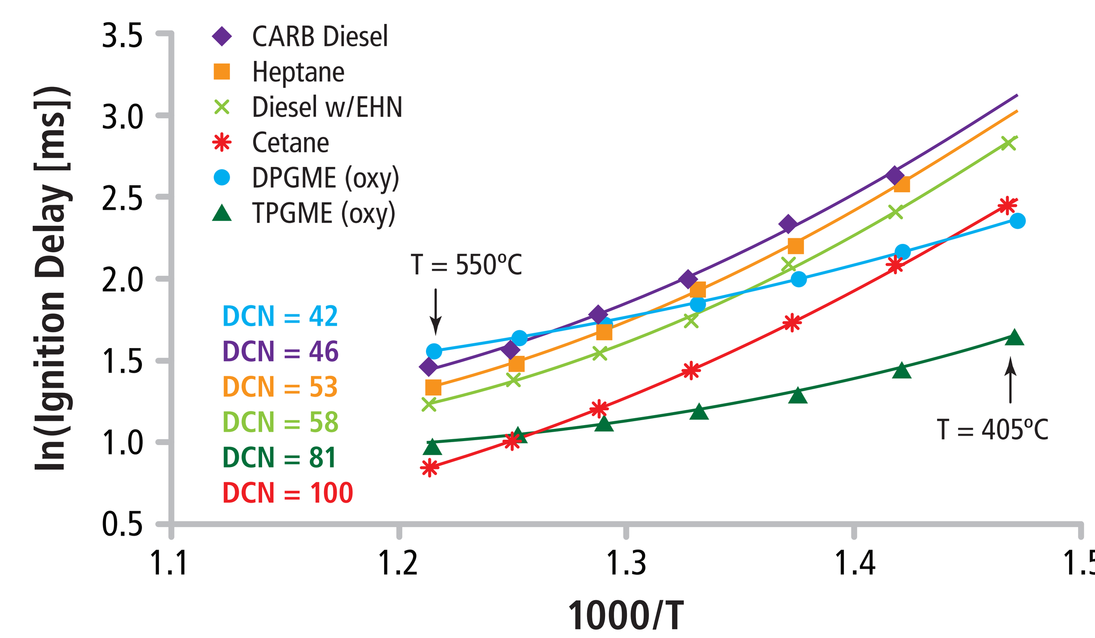
Ignition Quality Tester (IQT™)

- Constant volume spray combustion chamber
  - Requires ~50 mL fuel
- Ignition delay can be measured over a range of conditions:
  - T ~ 300 – 580°C
  - P ~ 5 – 30 bar
  - $[O_2]$: Up to 21% or beyond
    - Can measure derived cetane number (DCN) at specified conditions

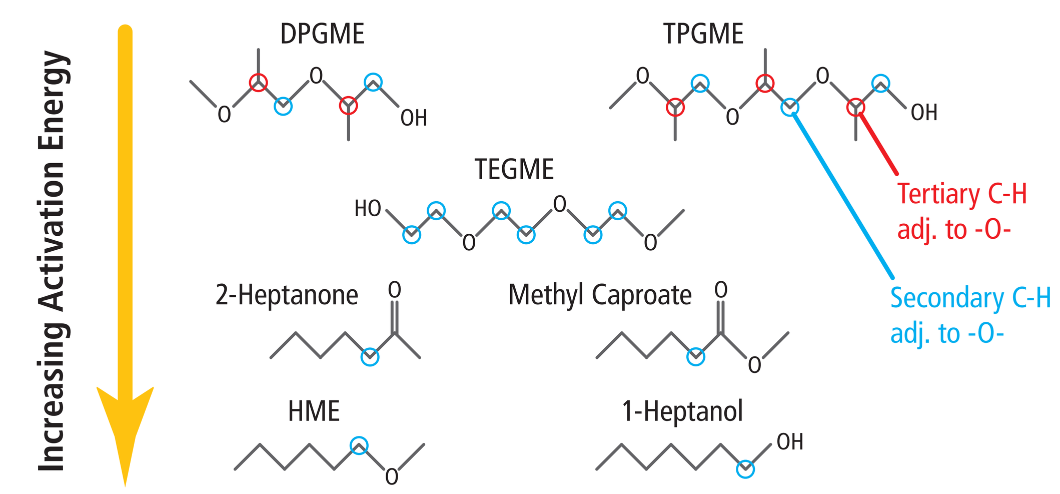


Experimental Data

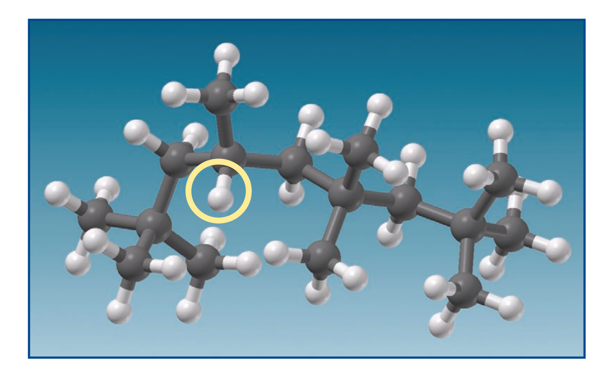
- Some oxygenates have a lower activation energy than normal hydrocarbons
  - Higher effective cetane number at reduced temperature
    - Cold-start implications
    - Impact on HCCI ignition

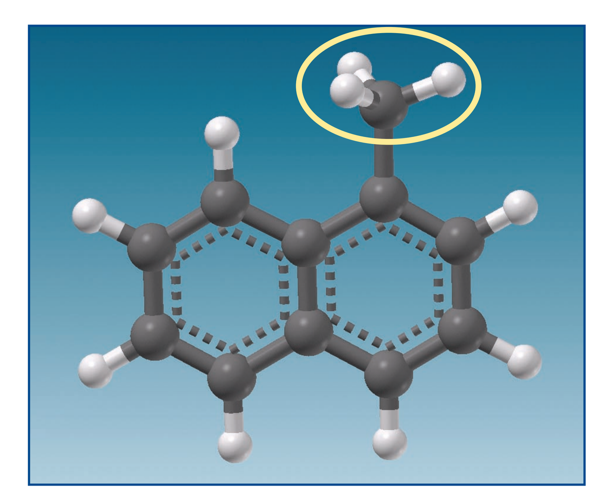


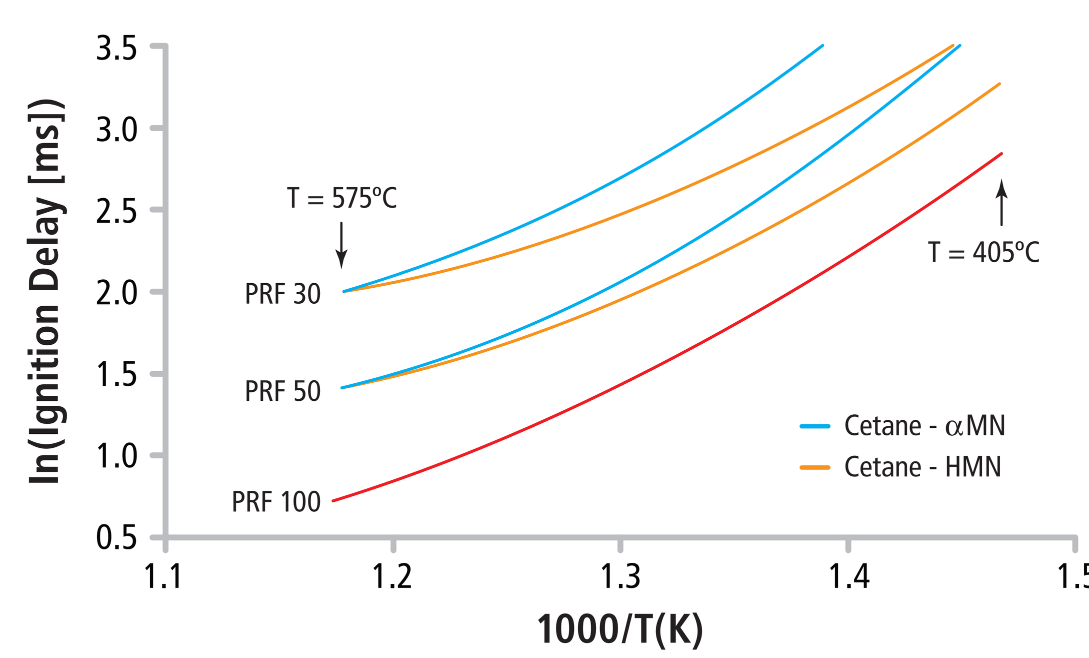
- Molecules with weakest C-H bonds have the lowest activation energy
  - Tertiary < Secondary < Primary
  - Adjacent to ether or carbonyl weaken C-H bonds



- Branching in hydrocarbons decreases activation energy
  - Tertiary C-H bonds
- Aromatic compounds increase activation energy
  - Resonance stabilization

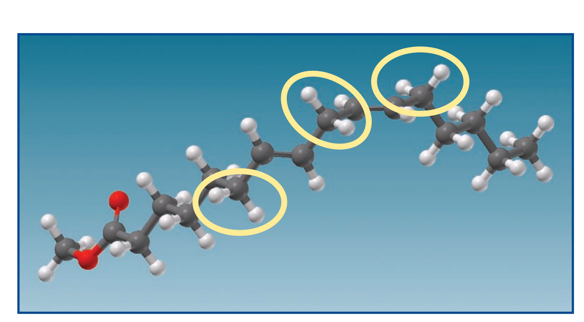


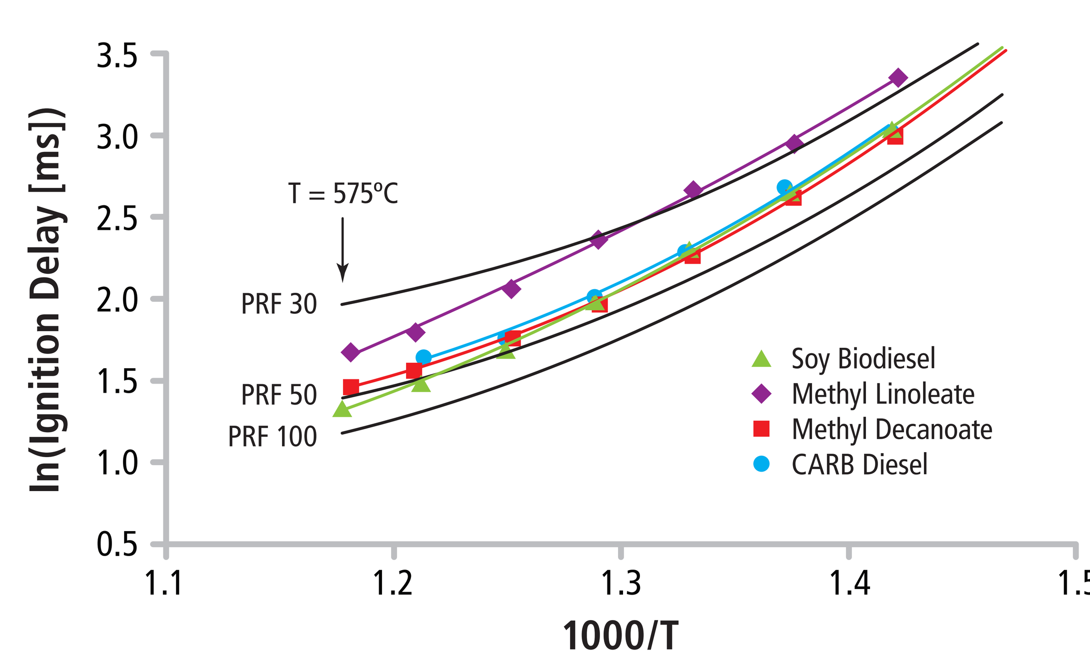




- Biodiesel fuels have a higher activation energy for ignition
  - Unsaturated bonds result in resonance-stabilized radicals

R• + O₂ ⇔ RO₂•

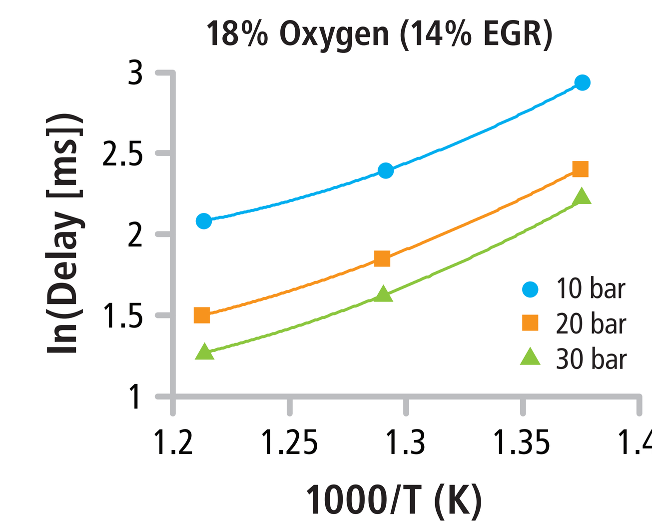




Analysis and Modeling

Fuel Sensitivity Parameters

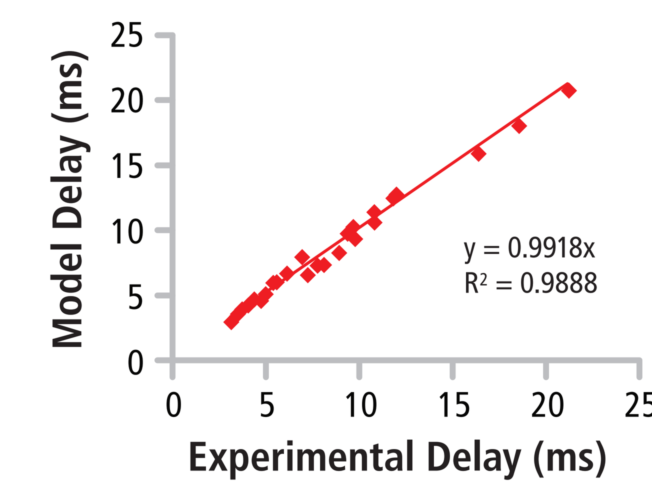
- Developed set of 27 points
  - T = 450, 500, 550 °C
  - P = 10, 20, 30 bar
  - $[O_2]$ = 15, 18, 21%



- Fit empirical rate model
  - To deconvolute $[O_2]$ and T effects

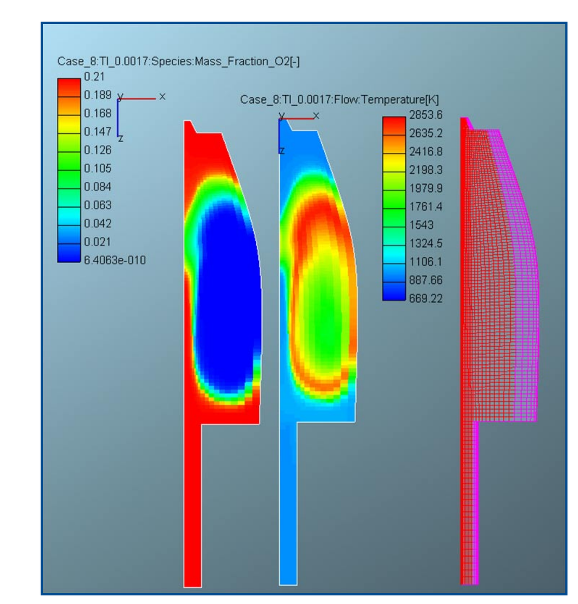
$$\text{Rate} = A \exp\left(\frac{-E_a}{RT}\right)[O_2]^b$$

Heptane: E_a = 50.2 kJ/mol, b = 0.74



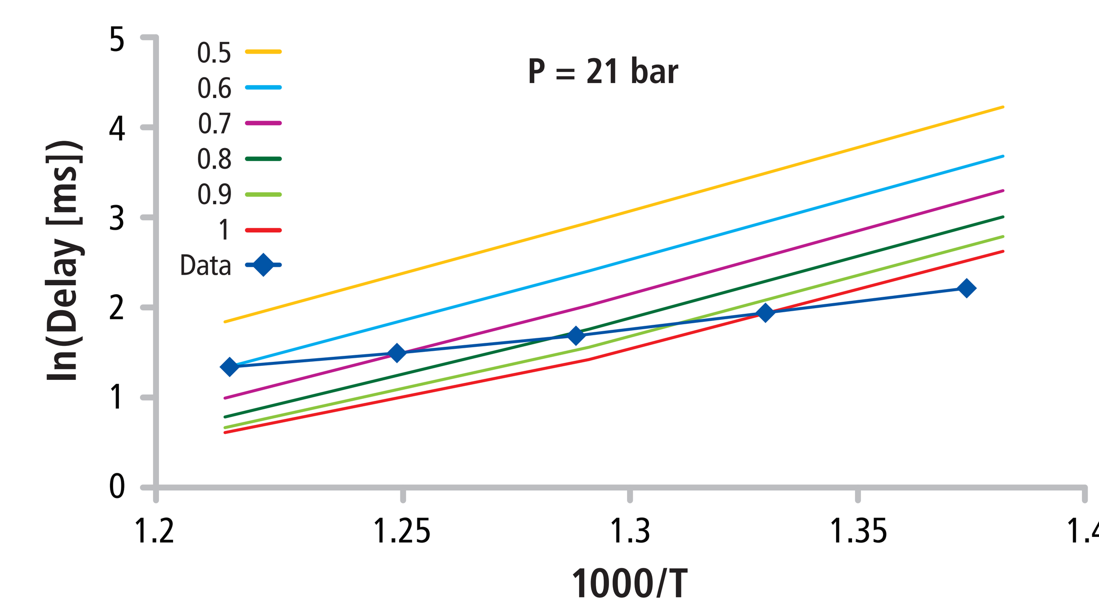
Integrated CFD Model of IQT™

- Spray: simplified cone model
- Evaporation and mixing
- Detailed chemistry w/ CHEMKIN
  - three mechanisms tested
- Ignition delays are too fast!



Mixing Factor Calculations

- Assumes fuel “perfectly” mixes with fraction of air in IQT
  - Ignores spray and mixing time
  - Accounts for temperature drop due to evaporation
- Data shows how mixing increases with ignition delay
  - Lower mixing factor as pressure increases for fixed delay



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